



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 04:00 PM UTC

PDB ID : 3UOI / pdb_00003uoi
Title : Mycobacterium tuberculosis bacterioferritin, BfrA
Authors : McMath, L.M.; Goulding, C.W.; TB Structural Genomics Consortium (TB-SGC)
Deposited on : 2011-11-16
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

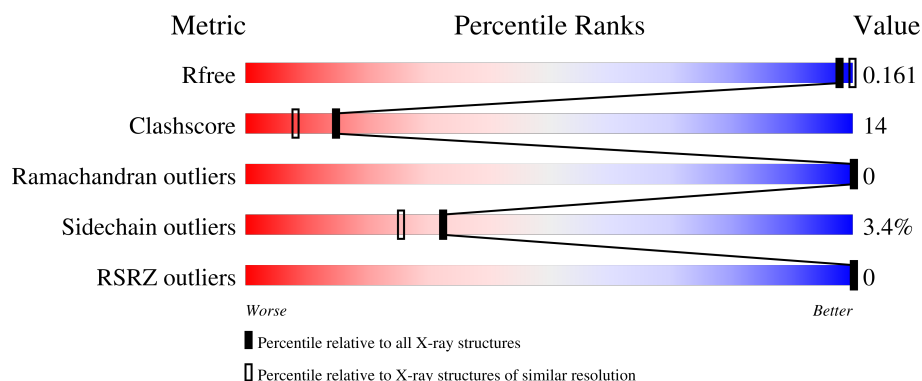
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



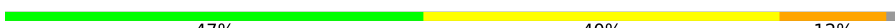
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	161	
1	B	161	
1	C	161	
1	D	161	
1	E	161	

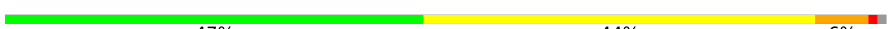
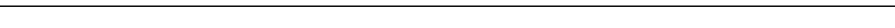
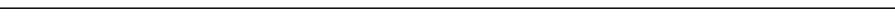
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Mol	Chain	Length	Quality of chain
1	F	161	 42% 47% 10% .
1	G	161	 37% 46% 16% .
1	H	161	 42% 47% 9% ..
1	I	161	 47% 40% 12% .
1	J	161	 49% 42% 8% .
1	K	161	 50% 43% 5% ..
1	L	161	 48% 43% 7% .
1	M	161	 48% 39% 12% ..
1	N	161	 42% 50% 6% ..
1	O	161	 47% 43% 9% .
1	P	161	 48% 38% 12% .
1	Q	161	 40% 45% 14% .
1	R	161	 52% 42% 5% .
1	S	161	 49% 35% 14% ..
1	T	161	 34% 53% 11% .
1	U	161	 45% 43% 11% ..
1	V	161	 50% 40% 8% .
1	W	161	 50% 38% 11% .
1	X	161	 45% 47% 6% ..
1	a	161	 45% 45% 7% ..
1	b	161	 39% 50% 10% .
1	c	161	 58% 34% 7% .
1	d	161	 55% 38% 5% ..
1	e	161	 50% 41% 8% .
1	f	161	 52% 40% 7% .

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Mol	Chain	Length	Quality of chain
1	g	161	 50% 43% 6% .
1	h	161	 54% 37% 7% .
1	i	161	 53% 34% 11% .
1	j	161	 51% 43% 5% .
1	k	161	 47% 44% 6% ..
1	l	161	 51% 43% 5% .
1	m	161	 40% 48% 9% ..
1	n	161	 43% 46% 10% .
1	o	161	 37% 46% 16% .
1	p	161	 47% 43% 9% .
1	q	161	 53% 34% 10% ..
1	r	161	 59% 34% 5% ..
1	s	161	 55% 39% 5% .
1	t	161	 42% 45% 11% ..
1	u	161	 39% 50% 11% .
1	v	161	 43% 45% 10% ..
1	w	161	 45% 41% 12% ..
1	x	161	 45% 45% 8% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEM	C	200	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 67560 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Bacterioferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	B	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	C	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	D	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	E	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	F	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	G	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	H	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	I	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	J	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	K	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	L	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	M	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	N	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	O	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	P	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	R	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	S	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	T	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	U	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	V	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	W	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	X	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	a	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	b	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	c	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	d	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	e	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	f	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	g	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	h	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	i	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	j	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	k	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	l	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	m	159	Total	C	N	O	S	0	0	0
			1281	800	218	256	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	n	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	o	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	p	159	Total	C	N	O	S	0	0	0
			1281	800	218	256	7			
1	q	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	r	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	s	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	t	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	u	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	v	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	w	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	x	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P63697
A	0	GLY	-	expression tag	UNP P63697
B	-1	MET	-	expression tag	UNP P63697
B	0	GLY	-	expression tag	UNP P63697
C	-1	MET	-	expression tag	UNP P63697
C	0	GLY	-	expression tag	UNP P63697
D	-1	MET	-	expression tag	UNP P63697
D	0	GLY	-	expression tag	UNP P63697
E	-1	MET	-	expression tag	UNP P63697
E	0	GLY	-	expression tag	UNP P63697
F	-1	MET	-	expression tag	UNP P63697
F	0	GLY	-	expression tag	UNP P63697
G	-1	MET	-	expression tag	UNP P63697
G	0	GLY	-	expression tag	UNP P63697
H	-1	MET	-	expression tag	UNP P63697
H	0	GLY	-	expression tag	UNP P63697
I	-1	MET	-	expression tag	UNP P63697

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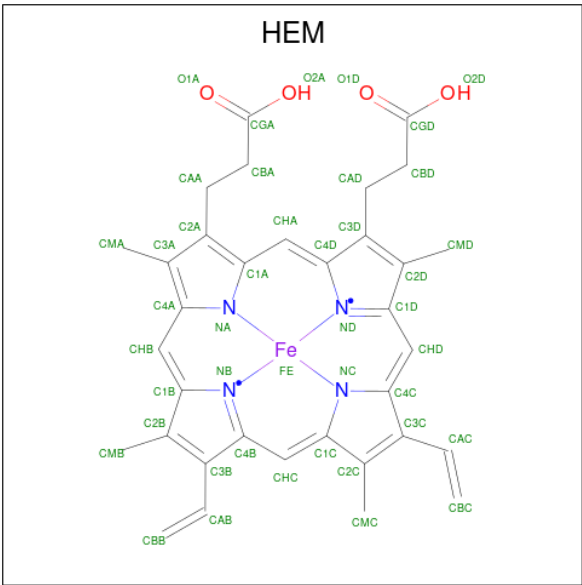
Chain	Residue	Modelled	Actual	Comment	Reference
I	0	GLY	-	expression tag	UNP P63697
J	-1	MET	-	expression tag	UNP P63697
J	0	GLY	-	expression tag	UNP P63697
K	-1	MET	-	expression tag	UNP P63697
K	0	GLY	-	expression tag	UNP P63697
L	-1	MET	-	expression tag	UNP P63697
L	0	GLY	-	expression tag	UNP P63697
M	-1	MET	-	expression tag	UNP P63697
M	0	GLY	-	expression tag	UNP P63697
N	-1	MET	-	expression tag	UNP P63697
N	0	GLY	-	expression tag	UNP P63697
O	-1	MET	-	expression tag	UNP P63697
O	0	GLY	-	expression tag	UNP P63697
P	-1	MET	-	expression tag	UNP P63697
P	0	GLY	-	expression tag	UNP P63697
Q	-1	MET	-	expression tag	UNP P63697
Q	0	GLY	-	expression tag	UNP P63697
R	-1	MET	-	expression tag	UNP P63697
R	0	GLY	-	expression tag	UNP P63697
S	-1	MET	-	expression tag	UNP P63697
S	0	GLY	-	expression tag	UNP P63697
T	-1	MET	-	expression tag	UNP P63697
T	0	GLY	-	expression tag	UNP P63697
U	-1	MET	-	expression tag	UNP P63697
U	0	GLY	-	expression tag	UNP P63697
V	-1	MET	-	expression tag	UNP P63697
V	0	GLY	-	expression tag	UNP P63697
W	-1	MET	-	expression tag	UNP P63697
W	0	GLY	-	expression tag	UNP P63697
X	-1	MET	-	expression tag	UNP P63697
X	0	GLY	-	expression tag	UNP P63697
a	-1	MET	-	expression tag	UNP P63697
a	0	GLY	-	expression tag	UNP P63697
b	-1	MET	-	expression tag	UNP P63697
b	0	GLY	-	expression tag	UNP P63697
c	-1	MET	-	expression tag	UNP P63697
c	0	GLY	-	expression tag	UNP P63697
d	-1	MET	-	expression tag	UNP P63697
d	0	GLY	-	expression tag	UNP P63697
e	-1	MET	-	expression tag	UNP P63697
e	0	GLY	-	expression tag	UNP P63697
f	-1	MET	-	expression tag	UNP P63697

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Chain	Residue	Modelled	Actual	Comment	Reference
f	0	GLY	-	expression tag	UNP P63697
g	-1	MET	-	expression tag	UNP P63697
g	0	GLY	-	expression tag	UNP P63697
h	-1	MET	-	expression tag	UNP P63697
h	0	GLY	-	expression tag	UNP P63697
i	-1	MET	-	expression tag	UNP P63697
i	0	GLY	-	expression tag	UNP P63697
j	-1	MET	-	expression tag	UNP P63697
j	0	GLY	-	expression tag	UNP P63697
k	-1	MET	-	expression tag	UNP P63697
k	0	GLY	-	expression tag	UNP P63697
l	-1	MET	-	expression tag	UNP P63697
l	0	GLY	-	expression tag	UNP P63697
m	-1	MET	-	expression tag	UNP P63697
m	0	GLY	-	expression tag	UNP P63697
n	-1	MET	-	expression tag	UNP P63697
n	0	GLY	-	expression tag	UNP P63697
o	-1	MET	-	expression tag	UNP P63697
o	0	GLY	-	expression tag	UNP P63697
p	-1	MET	-	expression tag	UNP P63697
p	0	GLY	-	expression tag	UNP P63697
q	-1	MET	-	expression tag	UNP P63697
q	0	GLY	-	expression tag	UNP P63697
r	-1	MET	-	expression tag	UNP P63697
r	0	GLY	-	expression tag	UNP P63697
s	-1	MET	-	expression tag	UNP P63697
s	0	GLY	-	expression tag	UNP P63697
t	-1	MET	-	expression tag	UNP P63697
t	0	GLY	-	expression tag	UNP P63697
u	-1	MET	-	expression tag	UNP P63697
u	0	GLY	-	expression tag	UNP P63697
v	-1	MET	-	expression tag	UNP P63697
v	0	GLY	-	expression tag	UNP P63697
w	-1	MET	-	expression tag	UNP P63697
w	0	GLY	-	expression tag	UNP P63697
x	-1	MET	-	expression tag	UNP P63697
x	0	GLY	-	expression tag	UNP P63697

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	M	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	R	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	S	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	X	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	a	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	c	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	g	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	j	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	k	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	n	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	o	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	t	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	v	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	x	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total 131	O 131	0	0
3	B	120	Total 120	O 120	0	0
3	C	89	Total 89	O 89	0	0
3	D	105	Total 105	O 105	0	0
3	E	104	Total 104	O 104	0	0
3	F	102	Total 102	O 102	0	0
3	G	115	Total 115	O 115	0	0
3	H	135	Total 135	O 135	0	0
3	I	127	Total 127	O 127	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	142	Total O 142 142	0	0
3	K	115	Total O 115 115	0	0
3	L	116	Total O 116 116	0	0
3	M	115	Total O 115 115	0	0
3	N	122	Total O 122 122	0	0
3	O	127	Total O 127 127	0	0
3	P	127	Total O 127 127	0	0
3	Q	108	Total O 108 108	0	0
3	R	104	Total O 104 104	0	0
3	S	73	Total O 73 73	0	0
3	T	136	Total O 136 136	0	0
3	U	151	Total O 151 151	0	0
3	V	119	Total O 119 119	0	0
3	W	91	Total O 91 91	0	0
3	X	131	Total O 131 131	0	0
3	a	65	Total O 65 65	0	0
3	b	59	Total O 59 59	0	0
3	c	94	Total O 94 94	0	0
3	d	57	Total O 57 57	0	0
3	e	103	Total O 103 103	0	0
3	f	105	Total O 105 105	0	0

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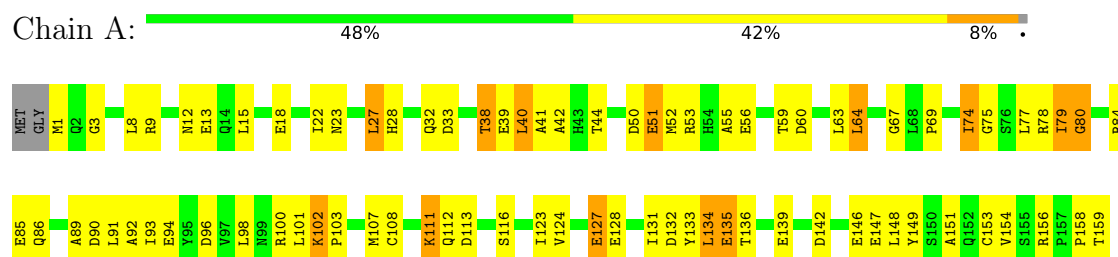
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	g	59	Total 59	O 59	0	0
3	h	63	Total 63	O 63	0	0
3	i	128	Total 128	O 128	0	0
3	j	74	Total 74	O 74	0	0
3	k	102	Total 102	O 102	0	0
3	l	120	Total 120	O 120	0	0
3	m	58	Total 58	O 58	0	0
3	n	41	Total 41	O 41	0	0
3	o	106	Total 106	O 106	0	0
3	p	69	Total 69	O 69	0	0
3	q	91	Total 91	O 91	0	0
3	r	96	Total 96	O 96	0	0
3	s	65	Total 65	O 65	0	0
3	t	69	Total 69	O 69	0	0
3	u	131	Total 131	O 131	0	0
3	v	74	Total 74	O 74	0	0
3	w	100	Total 100	O 100	0	0
3	x	122	Total 122	O 122	0	0

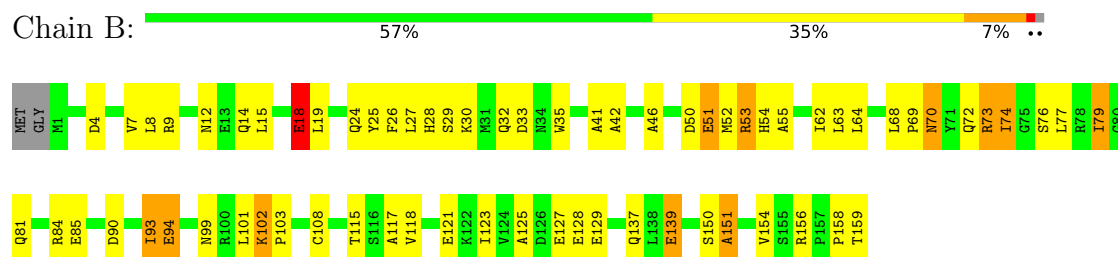
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

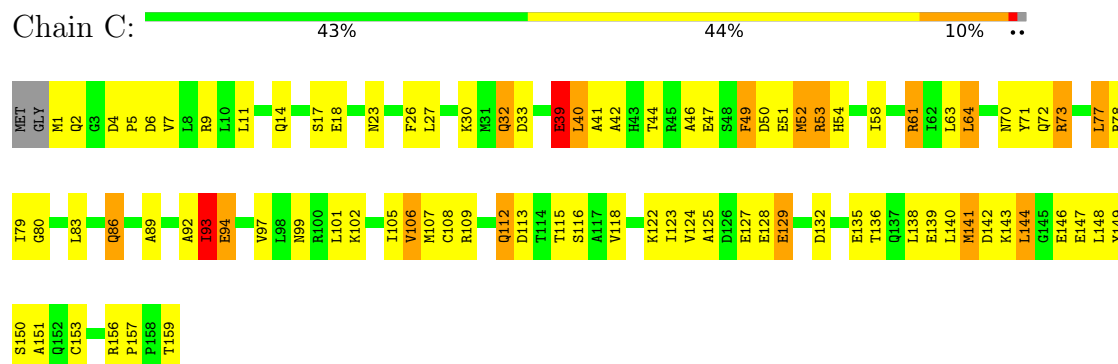
• Molecule 1: Bacterioferritin



• Molecule 1: Bacterioferritin

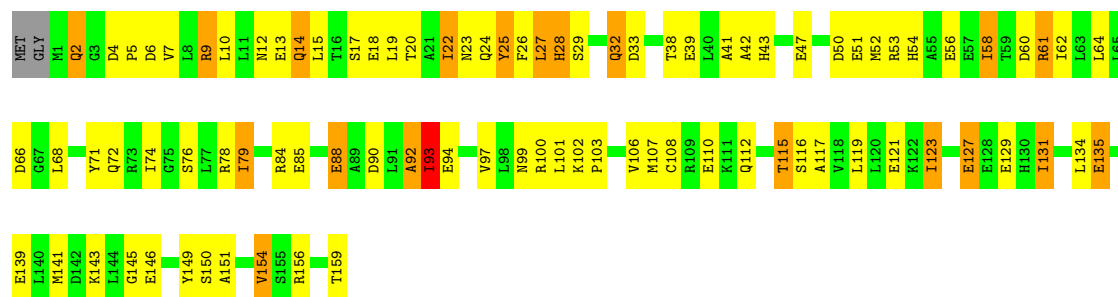


• Molecule 1: Bacterioferritin



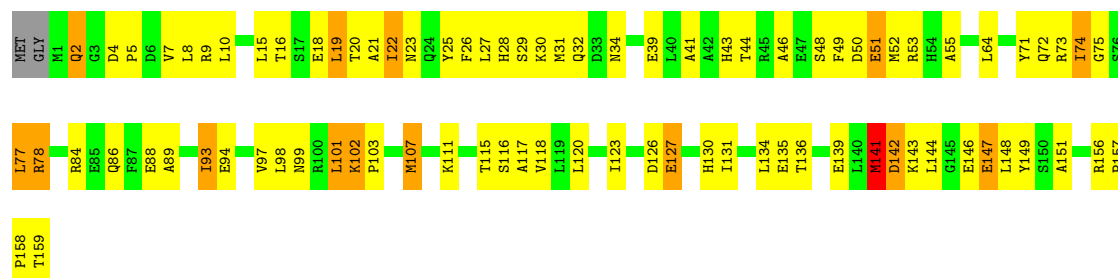
• Molecule 1: Bacterioferritin





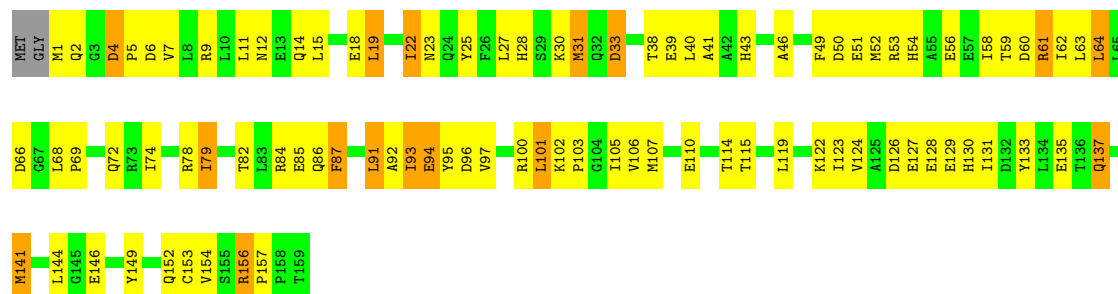
• Molecule 1: Bacterioferritin

Chain E: 46% 43% 9% ..



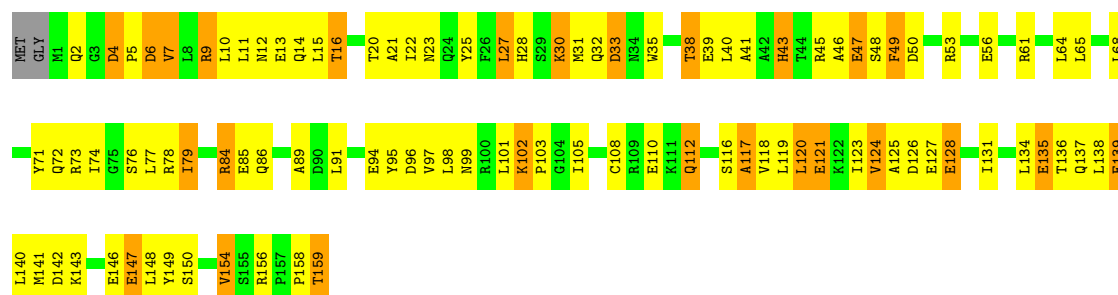
• Molecule 1: Bacterioferritin

Chain F: 42% 47% 10% .

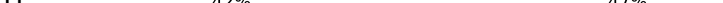


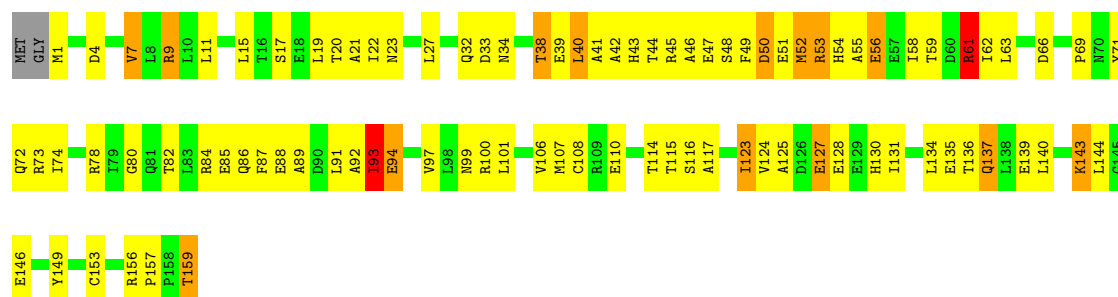
• Molecule 1: Bacterioferritin

Chain G: 37% 46% 16% .



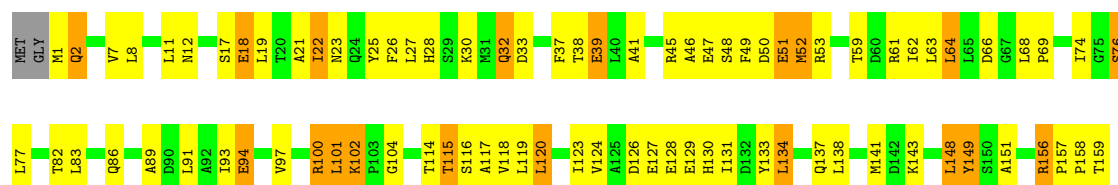
• Molecule 1: Bacterioferritin

Chain H:  42% 47% 9% ..

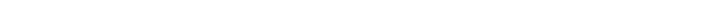


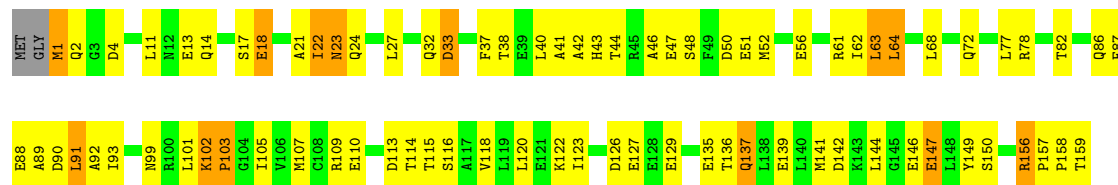
- Molecule 1: Bacterioferritin

Chain I: 47% 40% 12%

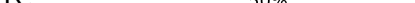


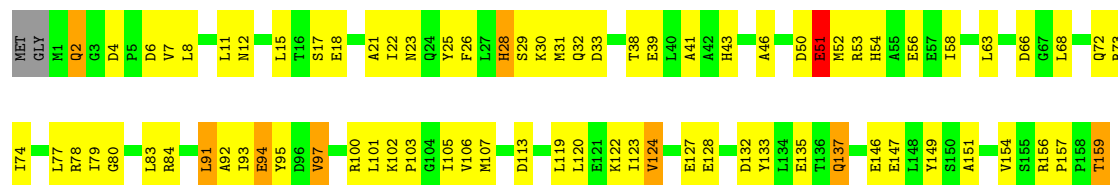
- Molecule 1: Bacterioferritin

Chain J:  49% 42% 8%

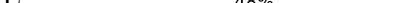


- Molecule 1: Bacterioferritin

Chain K:  50% 43% 5% ..



- Molecule 1: Bacterioferritin

Chain L:  48% 43% 7%

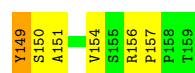




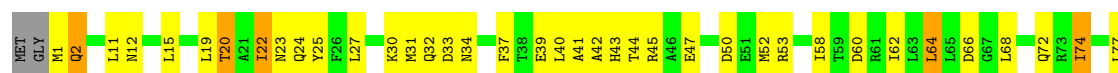
• Molecule 1: Bacterioferritin



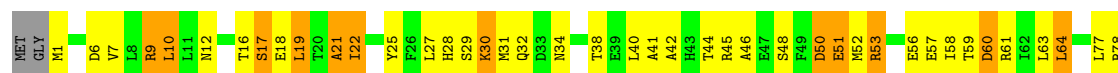
• Molecule 1: Bacterioferritin



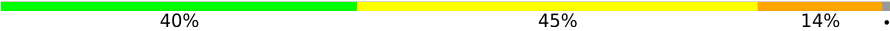
• Molecule 1: Bacterioferritin

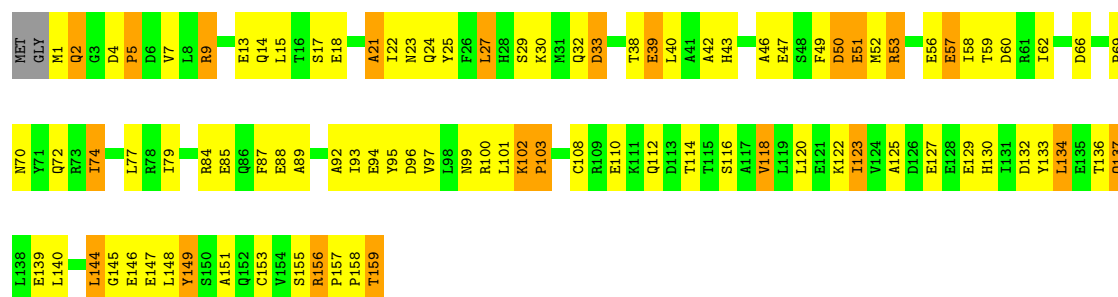


• Molecule 1: Bacterioferritin



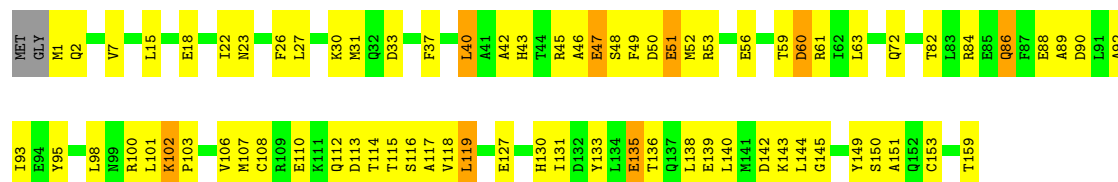
• Molecule 1: Bacterioferritin

Chain Q:  40% 45% 14% .

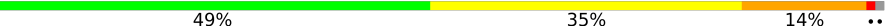


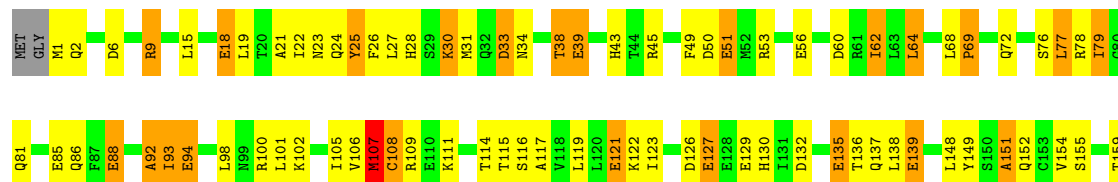
• Molecule 1: Bacterioferritin

Chain R:  52% 42% 5% .



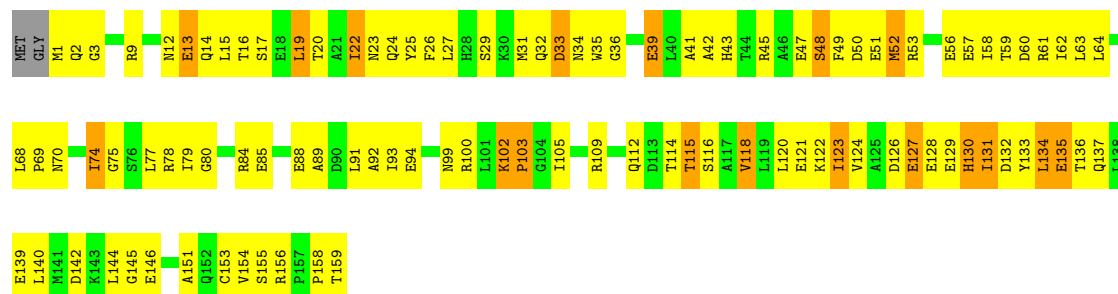
• Molecule 1: Bacterioferritin

Chain S:  49% 35% 14% ..



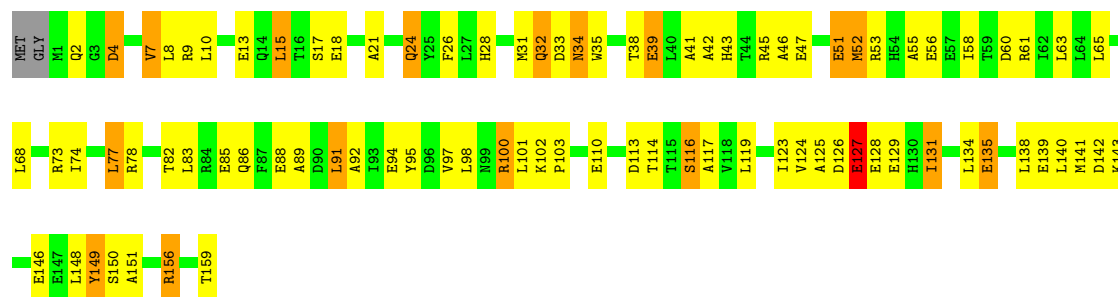
• Molecule 1: Bacterioferritin

Chain T:  34% 53% 11% .



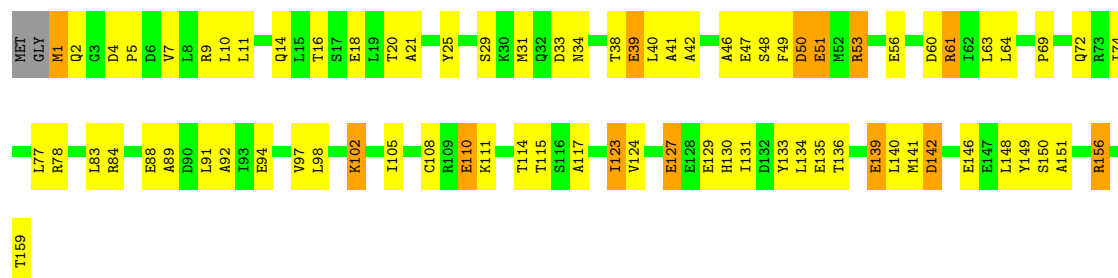
• Molecule 1: Bacterioferritin

Chain U:  45% 43% 11% ..



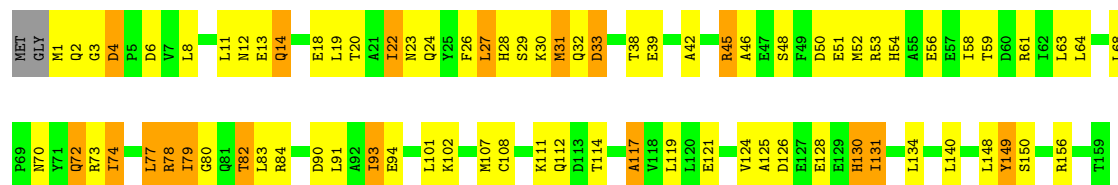
• Molecule 1: Bacterioferritin

Chain V: 50% 40% 8%



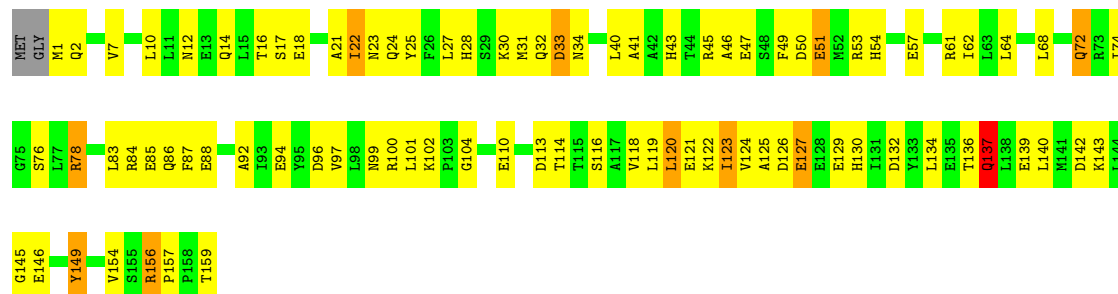
• Molecule 1: Bacterioferritin

Chain W: 50% 38% 11%



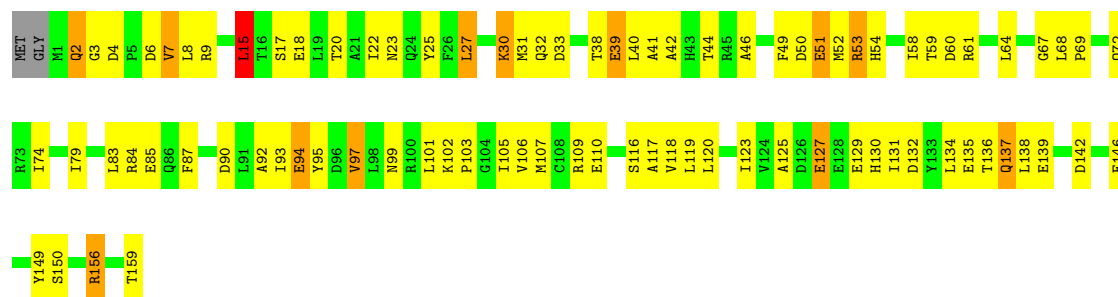
• Molecule 1: Bacterioferritin

Chain X: 45% 47% 6%



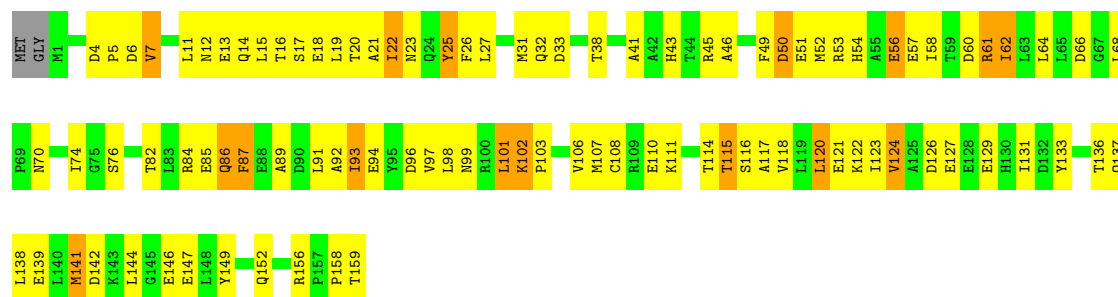
• Molecule 1: Bacterioferritin

Chain a: 45% 45% 7%



• Molecule 1: Bacterioferritin

Chain b: 39% 50% 10% .



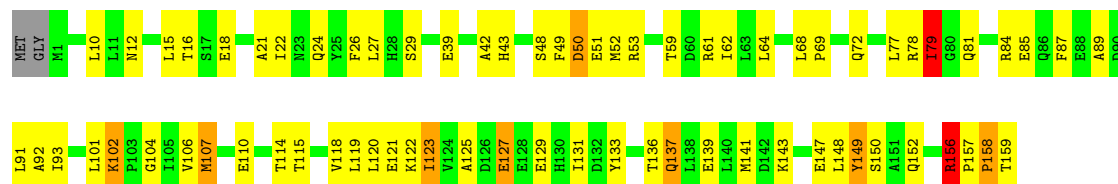
• Molecule 1: Bacterioferritin

Chain c: 58% 34% 7% .



• Molecule 1: Bacterioferritin

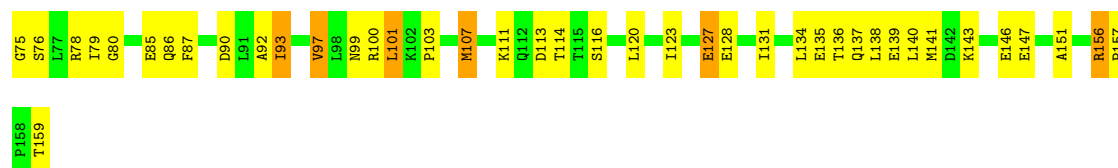
Chain d: 55% 38% 5% ..



• Molecule 1: Bacterioferritin

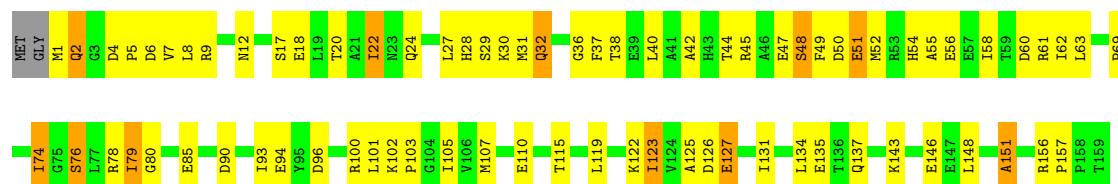
Chain e: 50% 41% 8% .





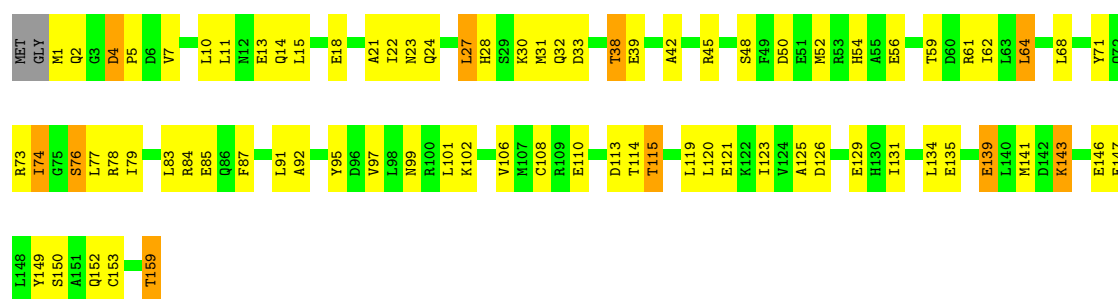
- Molecule 1: Bacterioferritin

Chain f: 52% 40% 7% .



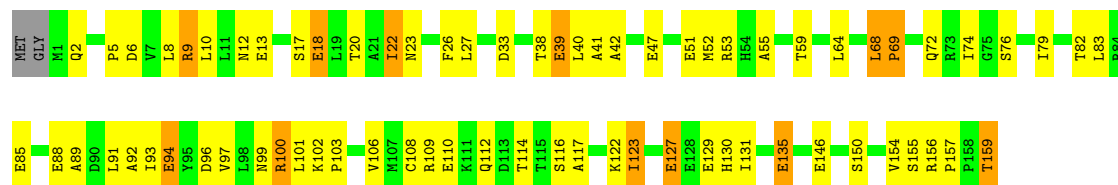
- Molecule 1: Bacterioferritin

Chain g: 50% 43% 6% .



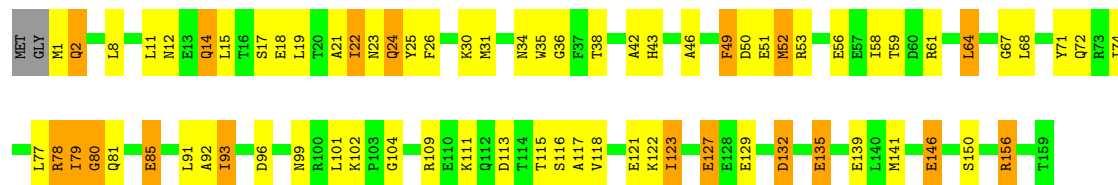
- Molecule 1: Bacterioferritin

Chain h: 54% 37% 7% .



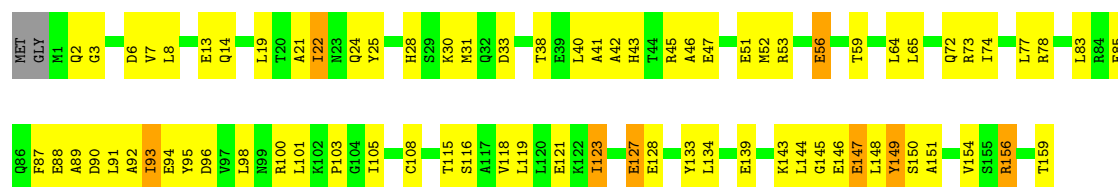
- Molecule 1: Bacterioferritin

Chain i: 53% 34% 11% .

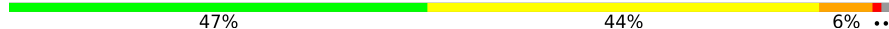


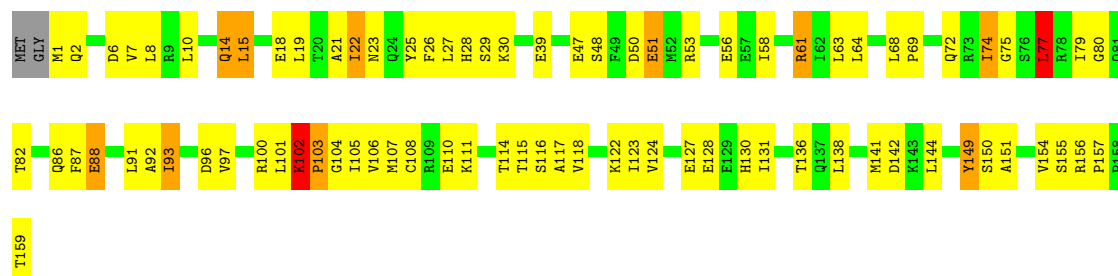
- Molecule 1: Bacterioferritin

Chain j:  51% 43% 5% .



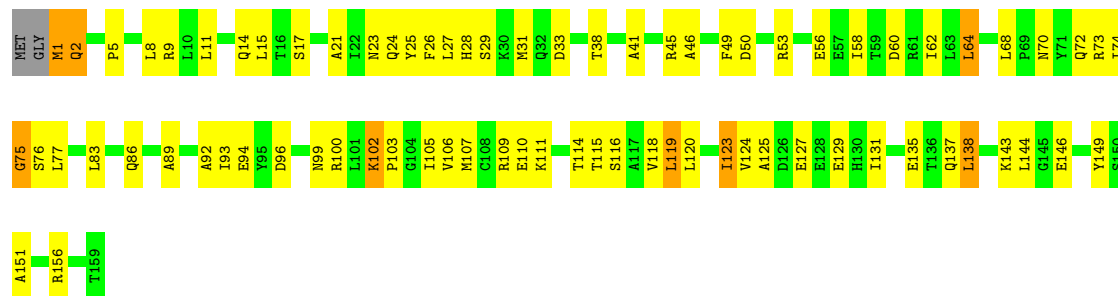
• Molecule 1: Bacterioferritin

Chain k:  47% 44% 6% ..



• Molecule 1: Bacterioferritin

Chain l:  51% 43% 5% .

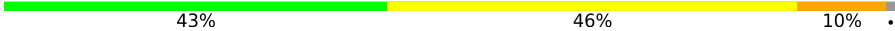


• Molecule 1: Bacterioferritin

Chain m:  40% 48% 9% ..



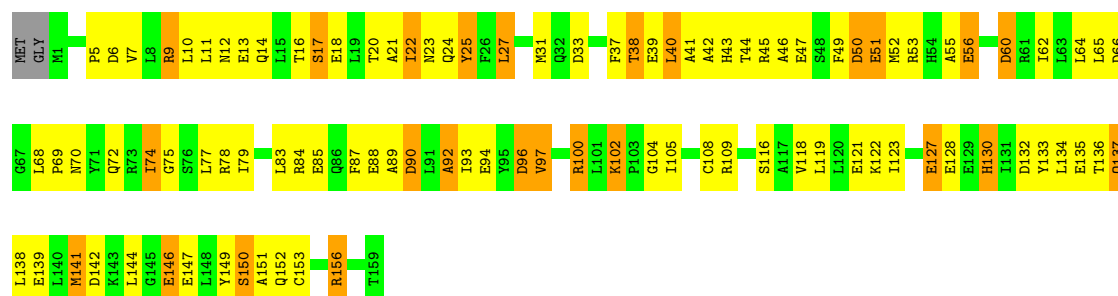
• Molecule 1: Bacterioferritin

Chain n: 



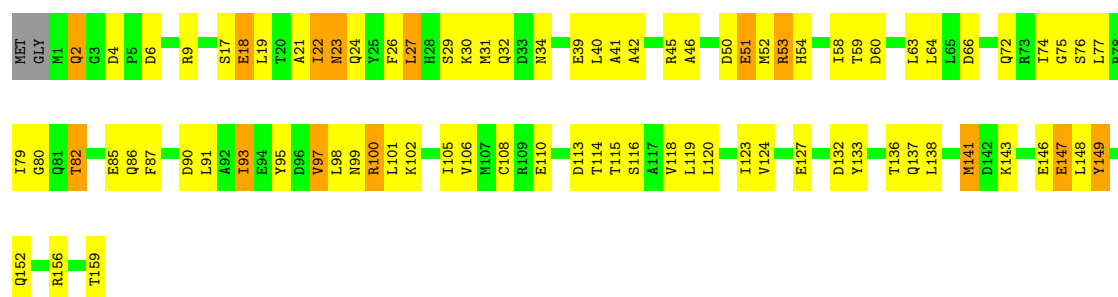
• Molecule 1: Bacterioferritin

Chain o: 



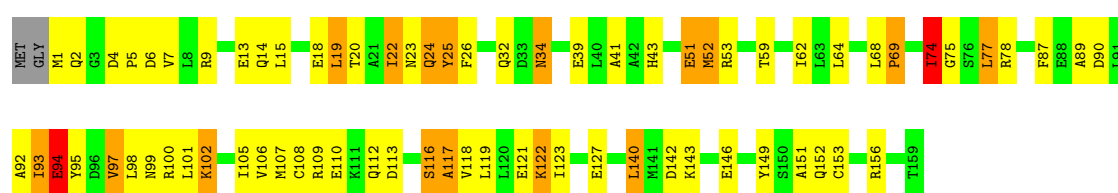
• Molecule 1: Bacterioferritin

Chain p: 



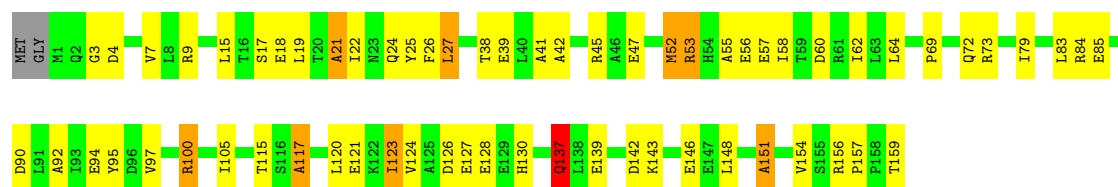
• Molecule 1: Bacterioferritin

Chain q: 



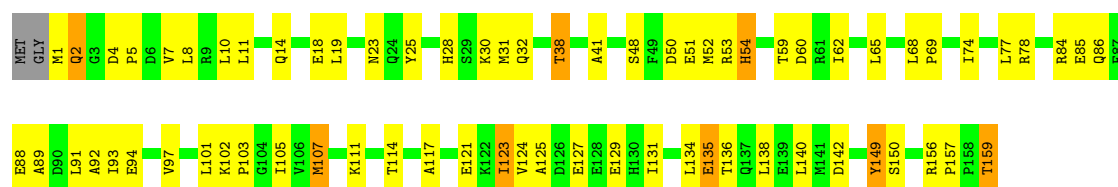
• Molecule 1: Bacterioferritin

Chain r: 

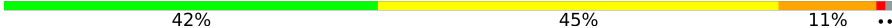


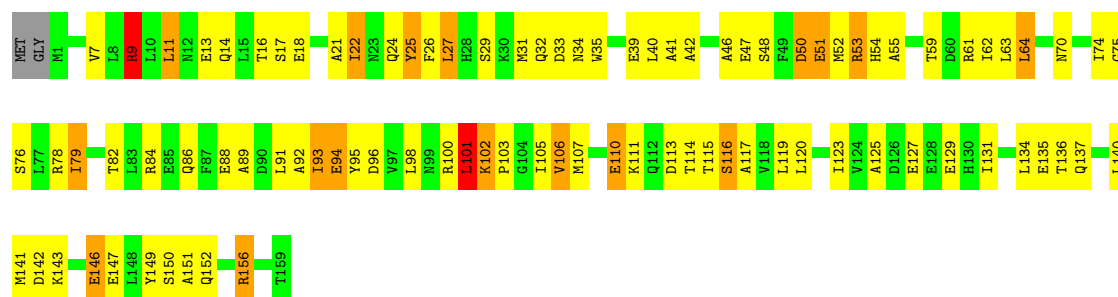
• Molecule 1: Bacterioferritin

Chain s: 



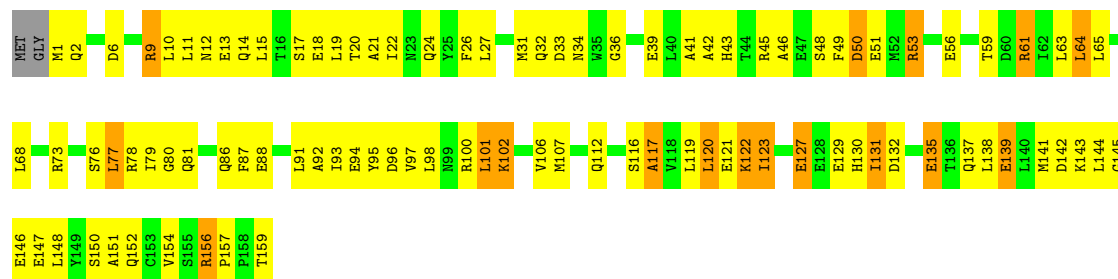
• Molecule 1: Bacterioferritin

Chain t: 

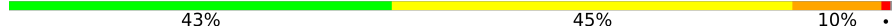


• Molecule 1: Bacterioferritin

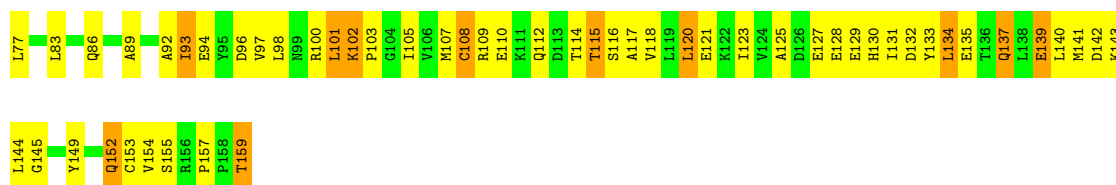
Chain u: 



• Molecule 1: Bacterioferritin

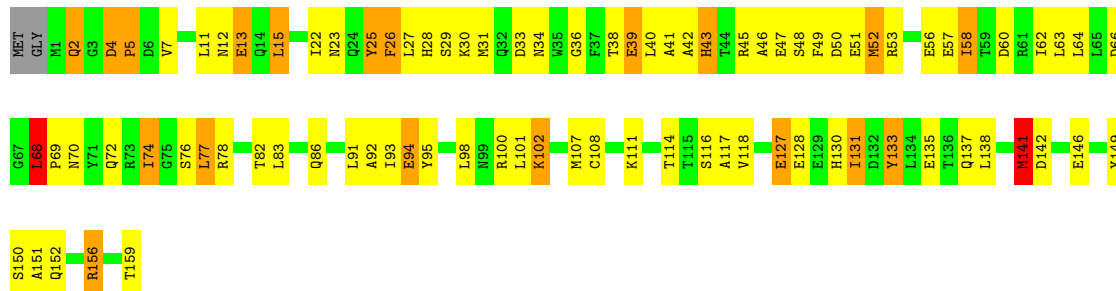
Chain v: 





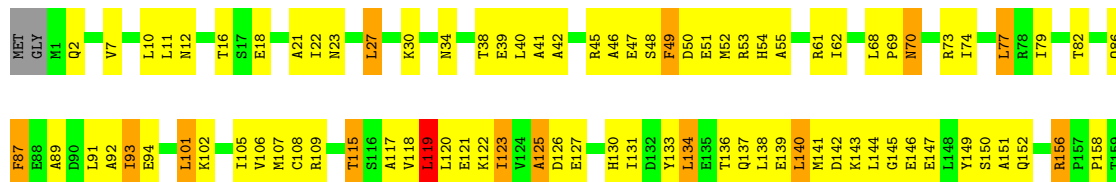
• Molecule 1: Bacterioferritin

Chain w: 45% 41% 12% ..



• Molecule 1: Bacterioferritin

Chain x: 45% 45% 8% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	122.96Å 123.22Å 175.45Å 89.95° 89.95° 90.00°	Depositor
Resolution (Å)	32.56 – 1.90 32.56 – 1.90	Depositor EDS
% Data completeness (in resolution range)	88.4 (32.56-1.90) 86.6 (32.56-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.148 , 0.194 0.162 , 0.161	Depositor DCC
R_{free} test set	35667 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 25.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.459 for k,-h,l 0.459 for -k,h,l 0.087 for h,-k,-l 0.087 for -h,k,-l 0.470 for -h,-k,l 0.087 for k,h,-l 0.087 for -k,-h,-l	Xtriage
Reported twinning fraction	0.315 for 1.000H, 1.000K, L 0.208 for -1.000H, -1.000K, L 0.232 for 1.000K, -1.000H, L 0.245 for -1.000K, 1.000H, L	Depositor
Outliers	0 of 718164 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	67560	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.20 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3586e-05.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.12	49/1304 (3.8%)	1.32	7/1763 (0.4%)
1	B	2.13	49/1304 (3.8%)	1.34	5/1763 (0.3%)
1	C	2.14	52/1304 (4.0%)	1.38	8/1763 (0.5%)
1	D	2.19	58/1304 (4.4%)	1.40	15/1763 (0.9%)
1	E	2.11	43/1304 (3.3%)	1.39	12/1763 (0.7%)
1	F	2.16	53/1304 (4.1%)	1.34	10/1763 (0.6%)
1	G	2.28	71/1304 (5.4%)	1.34	7/1763 (0.4%)
1	H	2.26	65/1304 (5.0%)	1.33	11/1763 (0.6%)
1	I	2.14	55/1304 (4.2%)	1.31	5/1763 (0.3%)
1	J	2.22	50/1304 (3.8%)	1.35	7/1763 (0.4%)
1	K	2.07	44/1304 (3.4%)	1.28	3/1763 (0.2%)
1	L	2.16	49/1304 (3.8%)	1.35	10/1763 (0.6%)
1	M	2.18	50/1304 (3.8%)	1.32	12/1763 (0.7%)
1	N	2.30	66/1304 (5.1%)	1.40	10/1763 (0.6%)
1	O	2.17	52/1304 (4.0%)	1.32	8/1763 (0.5%)
1	P	2.23	59/1304 (4.5%)	1.29	4/1763 (0.2%)
1	Q	2.19	56/1304 (4.3%)	1.33	5/1763 (0.3%)
1	R	2.10	37/1304 (2.8%)	1.40	13/1763 (0.7%)
1	S	2.22	62/1304 (4.8%)	1.40	8/1763 (0.5%)
1	T	2.32	77/1304 (5.9%)	1.28	5/1763 (0.3%)
1	U	2.30	71/1304 (5.4%)	1.37	11/1763 (0.6%)
1	V	2.17	57/1304 (4.4%)	1.32	4/1763 (0.2%)
1	W	2.15	47/1304 (3.6%)	1.36	9/1763 (0.5%)
1	X	2.22	64/1304 (4.9%)	1.34	9/1763 (0.5%)
1	a	2.31	63/1304 (4.8%)	1.32	8/1763 (0.5%)
1	b	2.27	71/1304 (5.4%)	1.33	5/1763 (0.3%)
1	c	2.06	31/1304 (2.4%)	1.38	10/1763 (0.6%)
1	d	2.09	41/1304 (3.1%)	1.32	8/1763 (0.5%)
1	e	2.02	40/1304 (3.1%)	1.36	7/1763 (0.4%)
1	f	2.09	44/1304 (3.4%)	1.36	9/1763 (0.5%)
1	g	2.18	53/1304 (4.1%)	1.33	4/1763 (0.2%)
1	h	2.10	45/1304 (3.5%)	1.29	7/1763 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	i	2.18	54/1304 (4.1%)	1.38	6/1763 (0.3%)
1	j	2.20	57/1304 (4.4%)	1.36	9/1763 (0.5%)
1	k	2.17	48/1304 (3.7%)	1.26	3/1763 (0.2%)
1	l	2.20	53/1304 (4.1%)	1.29	5/1763 (0.3%)
1	m	2.23	65/1300 (5.0%)	1.34	9/1758 (0.5%)
1	n	2.22	66/1304 (5.1%)	1.30	7/1763 (0.4%)
1	o	2.34	82/1304 (6.3%)	1.34	4/1763 (0.2%)
1	p	2.18	53/1300 (4.1%)	1.31	6/1758 (0.3%)
1	q	2.05	38/1304 (2.9%)	1.37	9/1763 (0.5%)
1	r	2.12	34/1304 (2.6%)	1.34	4/1763 (0.2%)
1	s	2.09	48/1304 (3.7%)	1.26	4/1763 (0.2%)
1	t	2.34	70/1304 (5.4%)	1.37	6/1763 (0.3%)
1	u	2.28	72/1304 (5.5%)	1.31	8/1763 (0.5%)
1	v	2.25	71/1304 (5.4%)	1.31	7/1763 (0.4%)
1	w	2.20	53/1304 (4.1%)	1.39	9/1763 (0.5%)
1	x	2.25	63/1304 (4.8%)	1.29	9/1763 (0.5%)
All	All	2.19	2651/62584 (4.2%)	1.34	361/84614 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	q	0	1

All (2651) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	93	ILE	C-N	17.98	1.55	1.33
1	f	127	GLU	C-N	15.72	1.54	1.33
1	p	51	GLU	C-N	14.45	1.52	1.33
1	E	127	GLU	C-N	12.51	1.50	1.33
1	J	18	GLU	C-N	11.29	1.48	1.33
1	t	25	TYR	C-N	-10.12	1.21	1.33
1	P	53	ARG	C-N	-10.11	1.20	1.33
1	E	126	ASP	C-N	-10.09	1.21	1.33
1	a	127	GLU	C-O	-9.96	1.12	1.24
1	l	151	ALA	C-O	-9.82	1.11	1.24
1	V	7	VAL	C-O	-9.62	1.13	1.24
1	i	52	MET	C-N	9.45	1.46	1.33
1	i	49	PHE	C-N	9.39	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	59	THR	C-O	-9.30	1.13	1.24
1	D	156	ARG	C-O	-9.29	1.17	1.25
1	a	53	ARG	C-O	-9.20	1.13	1.24
1	a	42	ALA	C-O	-9.10	1.13	1.24
1	J	46	ALA	CA-CB	-9.08	1.39	1.53
1	i	26	PHE	C-O	-9.05	1.13	1.24
1	r	41	ALA	C-O	-9.02	1.13	1.24
1	t	50	ASP	C-N	-9.00	1.22	1.33
1	L	123	ILE	C-O	-8.95	1.13	1.24
1	w	94	GLU	C-N	-8.94	1.22	1.33
1	x	102	LYS	C-O	-8.91	1.15	1.24
1	P	27	LEU	C-O	-8.83	1.13	1.24
1	x	7	VAL	C-O	-8.81	1.14	1.24
1	d	137	GLN	C-N	8.76	1.45	1.33
1	L	50	ASP	C-N	-8.73	1.22	1.34
1	o	123	ILE	C-O	-8.73	1.14	1.24
1	d	156	ARG	C-O	-8.72	1.17	1.25
1	G	156	ARG	C-O	-8.67	1.17	1.25
1	N	7	VAL	C-O	-8.66	1.14	1.24
1	G	14	GLN	C-O	-8.65	1.14	1.24
1	o	17	SER	C-O	-8.64	1.14	1.24
1	q	93	ILE	C-N	-8.62	1.23	1.33
1	M	60	ASP	C-O	-8.60	1.14	1.24
1	v	21	ALA	CA-CB	-8.60	1.39	1.53
1	U	55	ALA	CA-CB	-8.59	1.40	1.53
1	U	127	GLU	C-O	-8.57	1.14	1.24
1	e	51	GLU	C-N	8.52	1.45	1.33
1	q	108	CYS	C-O	-8.51	1.14	1.24
1	t	11	LEU	C-O	-8.48	1.14	1.24
1	g	24	GLN	C-O	-8.47	1.14	1.24
1	L	102	LYS	C-O	-8.46	1.16	1.24
1	t	89	ALA	C-O	-8.45	1.14	1.24
1	W	102	LYS	C-O	-8.42	1.16	1.24
1	X	102	LYS	C-O	-8.38	1.16	1.24
1	t	29	SER	C-O	-8.34	1.14	1.24
1	B	62	ILE	C-O	-8.34	1.14	1.24
1	o	156	ARG	C-O	-8.33	1.18	1.25
1	L	156	ARG	C-O	-8.33	1.17	1.25
1	a	102	LYS	C-O	-8.32	1.17	1.24
1	j	46	ALA	CA-CB	-8.28	1.40	1.53
1	n	56	GLU	C-O	-8.28	1.14	1.24
1	v	59	THR	C-O	-8.27	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	92	ALA	C-O	-8.27	1.14	1.24
1	k	8	LEU	C-O	-8.25	1.14	1.24
1	I	11	LEU	C-O	-8.25	1.14	1.24
1	x	140	LEU	C-O	-8.22	1.14	1.24
1	G	41	ALA	C-O	-8.21	1.14	1.24
1	W	124	VAL	C-O	-8.21	1.14	1.24
1	t	131	ILE	C-O	-8.20	1.14	1.24
1	m	156	ARG	C-O	-8.19	1.17	1.25
1	X	83	LEU	C-O	-8.16	1.14	1.24
1	M	156	ARG	C-O	-8.15	1.17	1.25
1	m	116	SER	C-O	-8.15	1.14	1.24
1	X	23	ASN	C-O	-8.14	1.14	1.24
1	D	93	ILE	C-N	8.13	1.44	1.34
1	S	102	LYS	C-O	-8.12	1.16	1.24
1	w	58	ILE	C-O	-8.10	1.14	1.24
1	B	68	LEU	C-O	-8.09	1.18	1.25
1	t	40	LEU	C-O	-8.08	1.14	1.24
1	V	10	LEU	C-O	-8.08	1.14	1.24
1	S	93	ILE	C-N	8.07	1.44	1.33
1	M	102	LYS	C-O	-8.05	1.17	1.24
1	K	68	LEU	C-O	-8.03	1.17	1.25
1	H	58	ILE	C-O	-8.03	1.14	1.24
1	c	105	ILE	C-O	-8.03	1.15	1.24
1	U	123	ILE	C-O	-8.02	1.14	1.24
1	s	102	LYS	C-O	-8.01	1.16	1.24
1	i	93	ILE	C-N	-8.00	1.22	1.33
1	G	16	THR	C-O	-7.99	1.14	1.24
1	o	102	LYS	C-O	-7.98	1.16	1.24
1	o	62	ILE	C-O	-7.97	1.14	1.24
1	a	136	THR	C-O	-7.96	1.14	1.24
1	h	68	LEU	C-O	-7.96	1.17	1.25
1	C	40	LEU	C-O	-7.95	1.15	1.24
1	b	51	GLU	C-O	-7.94	1.14	1.24
1	Q	58	ILE	C-O	-7.94	1.15	1.24
1	l	102	LYS	C-O	-7.94	1.17	1.24
1	h	40	LEU	C-O	-7.93	1.14	1.24
1	v	26	PHE	C-O	-7.92	1.15	1.24
1	S	64	LEU	C-O	-7.92	1.14	1.24
1	N	147	GLU	C-O	-7.91	1.14	1.24
1	n	132	ASP	C-O	-7.91	1.14	1.24
1	v	102	LYS	C-O	-7.91	1.17	1.24
1	F	52	MET	C-O	-7.90	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	68	LEU	C-O	-7.89	1.17	1.24
1	W	156	ARG	C-O	-7.89	1.17	1.25
1	N	131	ILE	C-O	-7.86	1.15	1.24
1	H	56	GLU	C-O	-7.85	1.15	1.24
1	N	92	ALA	C-O	-7.85	1.15	1.24
1	w	69	PRO	C-O	-7.84	1.15	1.23
1	o	27	LEU	C-O	-7.84	1.15	1.24
1	a	103	PRO	C-O	-7.83	1.15	1.24
1	h	150	SER	C-O	-7.82	1.15	1.24
1	e	23	ASN	C-O	-7.80	1.15	1.24
1	S	127	GLU	C-O	-7.80	1.15	1.24
1	b	68	LEU	C-O	-7.80	1.18	1.25
1	x	105	ILE	C-O	-7.80	1.15	1.24
1	V	102	LYS	C-O	-7.79	1.17	1.24
1	k	69	PRO	C-O	-7.79	1.14	1.23
1	J	21	ALA	CA-CB	-7.78	1.41	1.53
1	u	127	GLU	C-O	-7.78	1.15	1.24
1	q	122	LYS	C-O	-7.78	1.15	1.24
1	G	128	GLU	C-O	-7.76	1.15	1.24
1	w	15	LEU	C-O	-7.74	1.15	1.24
1	j	14	GLN	C-O	-7.72	1.15	1.24
1	V	14	GLN	C-O	-7.72	1.15	1.24
1	t	102	LYS	C-O	-7.72	1.17	1.24
1	C	129	GLU	C-O	-7.72	1.15	1.24
1	X	30	LYS	C-O	-7.71	1.15	1.24
1	H	21	ALA	CA-CB	-7.71	1.41	1.53
1	L	24	GLN	C-O	-7.71	1.15	1.24
1	o	13	GLU	C-O	-7.70	1.15	1.24
1	K	156	ARG	C-O	-7.69	1.18	1.25
1	x	27	LEU	C-O	-7.68	1.15	1.24
1	U	21	ALA	CA-CB	-7.68	1.41	1.53
1	g	102	LYS	C-O	-7.67	1.17	1.24
1	o	20	THR	C-O	-7.67	1.15	1.24
1	H	45	ARG	C-O	-7.67	1.15	1.24
1	H	51	GLU	C-O	-7.66	1.15	1.24
1	K	8	LEU	C-O	-7.65	1.15	1.24
1	w	7	VAL	C-O	-7.65	1.15	1.24
1	m	43	HIS	C-O	-7.64	1.15	1.24
1	u	64	LEU	C-O	-7.64	1.15	1.24
1	j	41	ALA	C-O	-7.63	1.15	1.24
1	p	156	ARG	C-O	-7.63	1.18	1.25
1	M	41	ALA	CA-CB	-7.61	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	g	15	LEU	C-O	-7.60	1.15	1.24
1	o	23	ASN	C-O	-7.59	1.15	1.24
1	i	11	LEU	C-O	-7.58	1.15	1.24
1	W	11	LEU	C-O	-7.57	1.15	1.24
1	b	15	LEU	C-O	-7.57	1.15	1.24
1	i	25	TYR	C-N	-7.56	1.24	1.33
1	i	34	ASN	C-O	-7.56	1.15	1.24
1	a	125	ALA	C-O	-7.55	1.15	1.24
1	l	137	GLN	C-O	-7.55	1.15	1.24
1	E	23	ASN	C-O	-7.55	1.15	1.24
1	C	151	ALA	CA-CB	-7.54	1.40	1.53
1	Q	60	ASP	C-O	-7.53	1.15	1.24
1	x	136	THR	C-O	-7.53	1.15	1.24
1	u	148	LEU	C-O	-7.53	1.15	1.24
1	m	68	LEU	C-O	-7.53	1.17	1.24
1	F	14	GLN	C-O	-7.51	1.15	1.24
1	a	116	SER	C-O	-7.50	1.15	1.24
1	h	17	SER	C-O	-7.49	1.15	1.24
1	H	116	SER	C-O	-7.47	1.15	1.24
1	A	44	THR	C-O	-7.47	1.15	1.24
1	P	57	GLU	C-O	-7.46	1.15	1.24
1	H	52	MET	C-O	-7.46	1.15	1.24
1	e	68	LEU	C-O	-7.45	1.18	1.25
1	E	15	LEU	C-O	-7.45	1.15	1.24
1	U	156	ARG	C-O	-7.44	1.18	1.25
1	d	149	TYR	C-N	-7.44	1.23	1.33
1	G	68	LEU	C-O	-7.44	1.17	1.24
1	K	7	VAL	C-O	-7.43	1.15	1.24
1	A	102	LYS	C-O	-7.43	1.17	1.24
1	b	102	LYS	C-O	-7.41	1.17	1.24
1	T	102	LYS	C-O	-7.41	1.17	1.24
1	b	116	SER	C-O	-7.40	1.15	1.24
1	u	17	SER	C-O	-7.40	1.15	1.24
1	o	147	GLU	C-O	-7.40	1.15	1.24
1	H	50	ASP	C-O	-7.38	1.15	1.24
1	o	43	HIS	C-O	-7.38	1.15	1.24
1	V	130	HIS	C-O	-7.37	1.15	1.24
1	o	116	SER	C-O	-7.37	1.15	1.24
1	m	60	ASP	C-O	-7.36	1.15	1.24
1	f	126	ASP	C-N	-7.36	1.24	1.33
1	M	116	SER	C-O	-7.36	1.15	1.24
1	m	75	GLY	C-O	-7.35	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	102	LYS	N-CA	-7.34	1.41	1.46
1	M	57	GLU	C-O	-7.34	1.15	1.24
1	a	46	ALA	CA-CB	-7.34	1.41	1.53
1	A	63	LEU	C-O	-7.33	1.15	1.24
1	r	47	GLU	C-O	-7.33	1.15	1.24
1	n	49	PHE	C-O	-7.32	1.15	1.24
1	W	108	CYS	C-O	-7.32	1.15	1.24
1	n	41	ALA	CA-CB	-7.32	1.41	1.53
1	X	25	TYR	C-O	-7.31	1.15	1.24
1	x	131	ILE	C-O	-7.31	1.15	1.24
1	Q	120	LEU	C-O	-7.30	1.15	1.24
1	u	147	GLU	C-O	-7.30	1.15	1.24
1	P	16	THR	C-O	-7.30	1.15	1.24
1	J	156	ARG	C-O	-7.28	1.18	1.25
1	W	20	THR	C-O	-7.28	1.15	1.24
1	U	43	HIS	C-O	-7.26	1.15	1.24
1	H	69	PRO	C-O	-7.26	1.15	1.23
1	O	79	ILE	C-O	-7.26	1.15	1.24
1	i	118	VAL	C-O	-7.26	1.15	1.24
1	U	89	ALA	CA-CB	-7.26	1.42	1.53
1	u	122	LYS	C-O	-7.26	1.15	1.24
1	u	73	ARG	C-O	-7.25	1.15	1.23
1	T	63	LEU	C-O	-7.25	1.15	1.24
1	J	103	PRO	C-O	-7.24	1.15	1.24
1	C	149	TYR	C-O	-7.24	1.15	1.24
1	R	46	ALA	CA-CB	-7.24	1.41	1.53
1	S	92	ALA	CA-CB	-7.23	1.42	1.53
1	c	41	ALA	C-O	-7.23	1.15	1.24
1	l	156	ARG	C-O	-7.23	1.18	1.25
1	r	156	ARG	C-O	-7.22	1.19	1.25
1	l	14	GLN	C-O	-7.22	1.15	1.24
1	g	50	ASP	C-O	-7.22	1.15	1.24
1	n	50	ASP	C-O	-7.22	1.15	1.24
1	w	22	ILE	C-O	-7.22	1.16	1.24
1	b	62	ILE	C-O	-7.20	1.15	1.24
1	E	130	HIS	C-O	-7.20	1.15	1.24
1	P	21	ALA	CA-CB	-7.20	1.42	1.53
1	X	132	ASP	C-O	-7.20	1.15	1.24
1	T	42	ALA	C-O	-7.19	1.15	1.24
1	b	74	ILE	C-O	-7.18	1.16	1.24
1	J	64	LEU	C-O	-7.18	1.15	1.24
1	j	22	ILE	C-O	-7.17	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	129	GLU	C-O	-7.17	1.15	1.24
1	b	12	ASN	C-O	-7.17	1.15	1.24
1	T	23	ASN	C-O	-7.17	1.15	1.24
1	c	86	GLN	C-O	-7.16	1.15	1.24
1	i	15	LEU	C-O	-7.16	1.15	1.24
1	s	129	GLU	C-O	-7.16	1.15	1.24
1	b	45	ARG	C-O	-7.16	1.15	1.24
1	t	46	ALA	CA-CB	-7.16	1.42	1.53
1	N	102	LYS	C-O	-7.15	1.17	1.24
1	b	41	ALA	C-O	-7.15	1.15	1.24
1	b	38	THR	C-O	-7.15	1.15	1.24
1	H	123	ILE	C-O	-7.14	1.15	1.24
1	S	45	ARG	C-O	-7.14	1.15	1.24
1	o	55	ALA	CA-CB	-7.14	1.42	1.53
1	Q	59	THR	C-O	-7.12	1.15	1.24
1	F	7	VAL	C-O	-7.12	1.16	1.24
1	R	27	LEU	C-O	-7.12	1.15	1.24
1	i	21	ALA	C-O	-7.12	1.15	1.24
1	u	95	TYR	C-O	-7.12	1.15	1.24
1	G	40	LEU	C-O	-7.12	1.15	1.24
1	u	39	GLU	C-O	-7.11	1.16	1.24
1	Q	108	CYS	C-O	-7.11	1.15	1.24
1	h	85	GLU	C-O	-7.11	1.15	1.24
1	D	17	SER	C-O	-7.10	1.15	1.24
1	E	115	THR	C-O	-7.10	1.15	1.24
1	S	115	THR	C-O	-7.10	1.15	1.24
1	F	49	PHE	C-O	-7.10	1.15	1.24
1	i	115	THR	C-O	-7.10	1.15	1.24
1	r	9	ARG	C-O	-7.09	1.15	1.24
1	o	135	GLU	C-O	-7.08	1.15	1.24
1	g	149	TYR	C-O	-7.08	1.15	1.24
1	B	139	GLU	C-O	-7.08	1.16	1.24
1	g	121	GLU	C-O	-7.08	1.15	1.24
1	A	147	GLU	C-O	-7.08	1.16	1.24
1	k	110	GLU	C-O	-7.07	1.15	1.24
1	s	136	THR	C-O	-7.07	1.15	1.24
1	O	31	MET	C-O	-7.07	1.15	1.24
1	G	125	ALA	CA-CB	-7.06	1.42	1.53
1	X	22	ILE	C-O	-7.06	1.16	1.24
1	A	92	ALA	C-O	-7.06	1.15	1.24
1	B	24	GLN	C-O	-7.06	1.16	1.24
1	b	60	ASP	C-O	-7.05	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	l	17	SER	C-O	-7.05	1.15	1.24
1	J	114	THR	C-O	-7.04	1.15	1.24
1	X	7	VAL	C-O	-7.04	1.15	1.24
1	n	134	LEU	C-O	-7.04	1.16	1.24
1	U	102	LYS	C-O	-7.04	1.17	1.24
1	X	96	ASP	C-O	-7.04	1.15	1.24
1	N	47	GLU	C-O	-7.04	1.15	1.24
1	Q	118	VAL	C-O	-7.03	1.15	1.24
1	T	14	GLN	C-O	-7.03	1.15	1.24
1	r	45	ARG	C-O	-7.02	1.16	1.24
1	u	92	ALA	CA-CB	-7.02	1.42	1.53
1	O	132	ASP	C-O	-7.02	1.16	1.24
1	U	46	ALA	C-O	-7.01	1.16	1.24
1	w	56	GLU	C-O	-7.01	1.16	1.24
1	F	68	LEU	C-O	-7.01	1.18	1.25
1	m	76	SER	C-O	-7.00	1.15	1.24
1	S	31	MET	C-O	-7.00	1.16	1.24
1	e	128	GLU	C-O	-7.00	1.16	1.24
1	l	138	LEU	C-O	-7.00	1.16	1.24
1	s	107	MET	C-O	-7.00	1.16	1.24
1	N	21	ALA	C-O	-7.00	1.16	1.24
1	w	26	PHE	C-O	-7.00	1.16	1.24
1	r	85	GLU	C-O	-6.99	1.16	1.24
1	j	128	GLU	C-O	-6.99	1.16	1.24
1	T	49	PHE	C-O	-6.99	1.16	1.24
1	M	94	GLU	C-N	6.99	1.43	1.33
1	Q	123	ILE	C-O	-6.99	1.16	1.24
1	L	39	GLU	C-O	-6.98	1.15	1.24
1	u	2	GLN	C-O	-6.98	1.16	1.24
1	i	156	ARG	C-O	-6.98	1.18	1.24
1	u	76	SER	C-O	-6.98	1.15	1.24
1	Q	51	GLU	C-O	-6.98	1.15	1.24
1	P	46	ALA	CA-CB	-6.97	1.41	1.53
1	p	27	LEU	C-O	-6.97	1.16	1.24
1	p	110	GLU	C-O	-6.97	1.16	1.24
1	t	32	GLN	C-O	-6.97	1.16	1.24
1	O	20	THR	C-O	-6.96	1.15	1.24
1	Q	27	LEU	C-O	-6.96	1.16	1.24
1	H	47	GLU	C-O	-6.96	1.16	1.24
1	O	47	GLU	C-O	-6.96	1.16	1.24
1	T	32	GLN	C-O	-6.96	1.16	1.24
1	T	123	ILE	C-O	-6.96	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	g	28	HIS	C-O	-6.95	1.16	1.24
1	b	20	THR	C-O	-6.95	1.16	1.24
1	F	92	ALA	C-O	-6.95	1.15	1.24
1	G	7	VAL	C-O	-6.95	1.16	1.24
1	N	50	ASP	C-O	-6.95	1.15	1.24
1	P	45	ARG	C-O	-6.94	1.16	1.24
1	L	126	ASP	C-O	-6.94	1.16	1.24
1	P	117	ALA	C-O	-6.94	1.16	1.24
1	x	68	LEU	C-O	-6.94	1.18	1.24
1	E	27	LEU	C-O	-6.93	1.16	1.24
1	T	20	THR	C-O	-6.93	1.15	1.24
1	a	90	ASP	C-O	-6.93	1.16	1.24
1	K	63	LEU	C-O	-6.93	1.16	1.24
1	I	94	GLU	C-O	-6.92	1.16	1.24
1	R	86	GLN	C-O	-6.92	1.15	1.24
1	X	32	GLN	C-O	-6.92	1.16	1.24
1	H	124	VAL	C-O	-6.92	1.16	1.24
1	t	92	ALA	C-O	-6.92	1.15	1.24
1	k	58	ILE	C-O	-6.91	1.16	1.24
1	t	142	ASP	C-O	-6.91	1.16	1.24
1	N	97	VAL	C-O	-6.90	1.16	1.24
1	S	15	LEU	C-O	-6.90	1.16	1.24
1	T	134	LEU	C-O	-6.90	1.16	1.24
1	f	105	ILE	C-O	-6.90	1.16	1.24
1	i	14	GLN	C-O	-6.90	1.16	1.24
1	t	63	LEU	C-O	-6.90	1.16	1.24
1	S	132	ASP	C-O	-6.89	1.16	1.24
1	U	124	VAL	C-O	-6.89	1.16	1.24
1	H	62	ILE	C-O	-6.88	1.16	1.24
1	N	115	THR	C-O	-6.88	1.16	1.24
1	X	43	HIS	C-O	-6.87	1.16	1.24
1	b	123	ILE	C-O	-6.87	1.16	1.24
1	E	46	ALA	C-O	-6.87	1.16	1.24
1	w	108	CYS	C-O	-6.87	1.16	1.24
1	G	49	PHE	C-O	-6.87	1.16	1.24
1	R	33	ASP	C-O	-6.87	1.16	1.24
1	o	47	GLU	C-O	-6.86	1.16	1.24
1	J	118	VAL	C-O	-6.86	1.16	1.24
1	k	97	VAL	C-O	-6.86	1.16	1.24
1	t	34	ASN	C-O	-6.86	1.16	1.24
1	t	42	ALA	C-O	-6.86	1.16	1.24
1	E	19	LEU	C-O	-6.86	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	7	VAL	C-O	-6.85	1.16	1.24
1	M	97	VAL	C-O	-6.85	1.16	1.24
1	p	18	GLU	C-O	-6.85	1.15	1.24
1	A	27	LEU	C-O	-6.84	1.16	1.24
1	I	156	ARG	C-O	-6.84	1.18	1.25
1	N	142	ASP	C-O	-6.84	1.16	1.24
1	q	105	ILE	C-O	-6.84	1.16	1.24
1	f	47	GLU	C-O	-6.84	1.16	1.24
1	k	56	GLU	C-O	-6.84	1.16	1.24
1	p	40	LEU	C-O	-6.84	1.16	1.24
1	h	156	ARG	C-O	-6.83	1.18	1.24
1	t	147	GLU	C-O	-6.83	1.16	1.24
1	V	127	GLU	C-O	-6.83	1.16	1.24
1	O	24	GLN	C-O	-6.83	1.16	1.24
1	u	68	LEU	C-O	-6.83	1.16	1.24
1	p	119	LEU	C-O	-6.83	1.16	1.24
1	t	53	ARG	C-O	-6.82	1.16	1.24
1	E	55	ALA	CA-CB	-6.82	1.42	1.53
1	r	148	LEU	C-O	-6.82	1.16	1.24
1	c	39	GLU	C-O	-6.82	1.16	1.24
1	b	118	VAL	C-O	-6.81	1.16	1.24
1	A	96	ASP	C-O	-6.81	1.16	1.24
1	U	89	ALA	C-O	-6.81	1.16	1.24
1	D	93	ILE	C-O	-6.81	1.16	1.24
1	H	61	ARG	C-O	-6.81	1.16	1.24
1	o	139	GLU	C-O	-6.81	1.16	1.24
1	n	17	SER	C-O	-6.81	1.16	1.24
1	L	72	GLN	C-O	-6.81	1.16	1.24
1	M	136	THR	C-O	-6.80	1.16	1.24
1	N	41	ALA	C-O	-6.80	1.16	1.24
1	I	69	PRO	C-O	-6.79	1.16	1.23
1	P	56	GLU	C-O	-6.79	1.16	1.24
1	X	40	LEU	C-O	-6.79	1.16	1.24
1	B	7	VAL	C-O	-6.79	1.16	1.24
1	N	63	LEU	C-O	-6.79	1.16	1.24
1	S	22	ILE	C-O	-6.79	1.16	1.24
1	C	118	VAL	C-O	-6.78	1.16	1.24
1	v	23	ASN	C-O	-6.78	1.16	1.24
1	b	122	LYS	C-O	-6.78	1.16	1.24
1	d	102	LYS	C-O	-6.78	1.18	1.24
1	K	2	GLN	C-O	-6.77	1.16	1.24
1	S	56	GLU	C-O	-6.77	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	137	GLN	C-O	-6.77	1.16	1.24
1	W	119	LEU	C-O	-6.77	1.16	1.24
1	j	74	ILE	C-O	-6.77	1.17	1.24
1	k	107	MET	C-O	-6.77	1.16	1.24
1	q	68	LEU	C-O	-6.77	1.16	1.24
1	F	110	GLU	C-O	-6.77	1.16	1.24
1	v	18	GLU	C-O	-6.77	1.16	1.24
1	N	15	LEU	C-O	-6.76	1.16	1.24
1	C	39	GLU	C-O	-6.76	1.16	1.24
1	t	13	GLU	C-N	-6.76	1.24	1.34
1	f	74	ILE	C-O	-6.76	1.16	1.23
1	p	41	ALA	CA-CB	-6.76	1.42	1.53
1	m	46	ALA	CA-CB	-6.75	1.42	1.53
1	M	83	LEU	C-O	-6.74	1.16	1.24
1	b	50	ASP	C-N	-6.74	1.24	1.33
1	g	59	THR	C-O	-6.74	1.16	1.24
1	x	16	THR	C-O	-6.74	1.16	1.24
1	B	150	SER	C-O	-6.74	1.15	1.24
1	O	102	LYS	C-O	-6.74	1.18	1.24
1	U	31	MET	C-O	-6.74	1.16	1.24
1	R	151	ALA	CA-CB	-6.73	1.41	1.53
1	a	60	ASP	C-O	-6.73	1.16	1.24
1	q	87	PHE	C-O	-6.73	1.16	1.24
1	r	97	VAL	C-O	-6.72	1.16	1.24
1	Q	29	SER	C-O	-6.71	1.16	1.24
1	j	115	THR	C-O	-6.71	1.16	1.24
1	C	54	HIS	C-O	-6.71	1.16	1.24
1	j	156	ARG	C-O	-6.71	1.18	1.24
1	E	136	THR	C-O	-6.71	1.16	1.24
1	d	27	LEU	C-O	-6.71	1.16	1.24
1	d	106	VAL	C-O	-6.70	1.16	1.24
1	T	127	GLU	C-O	-6.70	1.16	1.24
1	P	116	SER	C-O	-6.70	1.16	1.24
1	W	42	ALA	CA-CB	-6.70	1.42	1.53
1	e	139	GLU	C-O	-6.70	1.16	1.24
1	F	15	LEU	C-O	-6.69	1.16	1.24
1	F	119	LEU	C-O	-6.69	1.16	1.24
1	N	9	ARG	C-O	-6.69	1.16	1.24
1	u	43	HIS	C-O	-6.69	1.16	1.24
1	d	122	LYS	C-O	-6.68	1.16	1.24
1	g	74	ILE	C-O	-6.68	1.16	1.23
1	N	117	ALA	CA-CB	-6.68	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	q	7	VAL	C-O	-6.68	1.16	1.24
1	u	119	LEU	C-O	-6.67	1.16	1.24
1	j	21	ALA	CA-CB	-6.67	1.42	1.53
1	q	89	ALA	C-O	-6.67	1.16	1.24
1	V	129	GLU	C-O	-6.67	1.16	1.24
1	T	99	ASN	C-O	-6.66	1.16	1.24
1	n	115	THR	C-O	-6.66	1.16	1.24
1	I	59	THR	C-O	-6.66	1.16	1.24
1	E	20	THR	C-O	-6.65	1.16	1.24
1	K	102	LYS	C-O	-6.65	1.18	1.24
1	N	100	ARG	C-O	-6.65	1.16	1.24
1	U	60	ASP	C-O	-6.65	1.16	1.24
1	r	64	LEU	C-O	-6.65	1.16	1.24
1	q	95	TYR	C-O	-6.65	1.16	1.24
1	A	85	GLU	C-O	-6.65	1.16	1.24
1	M	27	LEU	C-O	-6.65	1.16	1.24
1	l	114	THR	C-O	-6.65	1.16	1.24
1	p	32	GLN	C-O	-6.64	1.16	1.24
1	u	86	GLN	C-O	-6.64	1.16	1.24
1	b	120	LEU	C-O	-6.64	1.16	1.24
1	n	26	PHE	C-O	-6.64	1.16	1.24
1	A	84	ARG	C-O	-6.64	1.16	1.24
1	e	9	ARG	C-O	-6.64	1.16	1.24
1	V	105	ILE	C-O	-6.63	1.16	1.24
1	T	51	GLU	C-O	-6.63	1.16	1.24
1	l	125	ALA	C-O	-6.63	1.16	1.24
1	H	127	GLU	C-O	-6.63	1.16	1.24
1	g	125	ALA	CA-CB	-6.63	1.43	1.53
1	c	27	LEU	C-O	-6.62	1.16	1.24
1	F	96	ASP	C-O	-6.62	1.16	1.24
1	T	50	ASP	C-O	-6.62	1.16	1.24
1	T	60	ASP	C-O	-6.62	1.16	1.24
1	q	99	ASN	C-O	-6.62	1.16	1.24
1	w	23	ASN	C-O	-6.62	1.16	1.24
1	G	39	GLU	C-O	-6.62	1.16	1.24
1	T	92	ALA	C-O	-6.62	1.16	1.24
1	b	114	THR	C-O	-6.62	1.16	1.24
1	k	7	VAL	C-O	-6.62	1.16	1.24
1	V	31	MET	C-O	-6.62	1.16	1.24
1	m	125	ALA	C-O	-6.62	1.16	1.24
1	m	102	LYS	C-O	-6.62	1.18	1.24
1	D	24	GLN	C-O	-6.61	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	108	CYS	C-O	-6.61	1.16	1.24
1	X	54	HIS	C-O	-6.61	1.16	1.24
1	A	75	GLY	C-O	-6.61	1.15	1.23
1	w	27	LEU	C-O	-6.61	1.16	1.24
1	T	64	LEU	C-O	-6.61	1.16	1.24
1	s	31	MET	C-O	-6.61	1.16	1.24
1	D	25	TYR	C-O	-6.60	1.16	1.24
1	o	42	ALA	CA-CB	-6.60	1.43	1.53
1	l	24	GLN	C-O	-6.60	1.16	1.24
1	t	137	GLN	C-O	-6.60	1.16	1.24
1	v	110	GLU	C-O	-6.60	1.15	1.24
1	u	138	LEU	C-O	-6.60	1.16	1.24
1	e	127	GLU	C-O	-6.60	1.16	1.24
1	V	123	ILE	C-O	-6.59	1.16	1.24
1	t	25	TYR	C-O	-6.59	1.16	1.24
1	c	41	ALA	CA-CB	-6.59	1.43	1.53
1	L	125	ALA	C-O	-6.59	1.16	1.24
1	G	30	LYS	C-O	-6.59	1.16	1.24
1	B	76	SER	C-O	-6.58	1.16	1.24
1	H	21	ALA	C-O	-6.58	1.16	1.24
1	g	21	ALA	C-O	-6.58	1.16	1.24
1	o	134	LEU	C-O	-6.58	1.16	1.24
1	e	26	PHE	C-O	-6.58	1.16	1.24
1	v	141	MET	C-O	-6.58	1.16	1.24
1	H	39	GLU	C-O	-6.58	1.16	1.24
1	P	19	LEU	C-O	-6.58	1.16	1.24
1	R	135	GLU	C-O	-6.57	1.16	1.24
1	S	107	MET	SD-CE	-6.57	1.63	1.79
1	t	114	THR	C-O	-6.57	1.16	1.24
1	O	92	ALA	C-O	-6.56	1.16	1.24
1	j	139	GLU	C-O	-6.56	1.16	1.24
1	F	156	ARG	C-O	-6.56	1.18	1.24
1	a	32	GLN	C-O	-6.56	1.16	1.24
1	x	54	HIS	C-O	-6.56	1.16	1.24
1	o	44	THR	C-O	-6.55	1.16	1.24
1	x	108	CYS	C-O	-6.55	1.16	1.24
1	b	22	ILE	C-O	-6.55	1.16	1.24
1	J	122	LYS	C-O	-6.55	1.16	1.24
1	I	26	PHE	C-O	-6.55	1.16	1.24
1	X	156	ARG	C-O	-6.55	1.18	1.24
1	m	83	LEU	C-O	-6.55	1.16	1.24
1	J	137	GLN	C-O	-6.55	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	136	THR	C-O	-6.54	1.16	1.24
1	V	89	ALA	CA-CB	-6.54	1.43	1.53
1	a	74	ILE	C-O	-6.54	1.17	1.24
1	t	22	ILE	C-O	-6.54	1.16	1.24
1	T	89	ALA	C-O	-6.54	1.16	1.24
1	J	147	GLU	C-O	-6.53	1.16	1.24
1	V	53	ARG	C-O	-6.53	1.16	1.24
1	V	72	GLN	C-O	-6.53	1.16	1.24
1	S	34	ASN	C-O	-6.53	1.16	1.24
1	o	152	GLN	C-O	-6.53	1.15	1.24
1	o	74	ILE	C-O	-6.53	1.17	1.24
1	p	19	LEU	C-O	-6.53	1.16	1.24
1	U	13	GLU	C-O	-6.52	1.16	1.24
1	n	97	VAL	C-O	-6.52	1.16	1.24
1	Q	43	HIS	C-O	-6.52	1.16	1.24
1	t	129	GLU	C-O	-6.52	1.16	1.24
1	x	41	ALA	CA-CB	-6.52	1.43	1.53
1	v	96	ASP	C-O	-6.52	1.16	1.24
1	L	27	LEU	C-O	-6.51	1.16	1.24
1	S	30	LYS	C-O	-6.51	1.16	1.24
1	J	37	PHE	C-O	-6.51	1.14	1.23
1	v	45	ARG	C-O	-6.51	1.16	1.24
1	T	39	GLU	C-O	-6.50	1.16	1.24
1	t	107	MET	C-O	-6.50	1.16	1.24
1	I	25	TYR	C-O	-6.50	1.16	1.24
1	D	27	LEU	C-O	-6.50	1.16	1.24
1	Q	62	ILE	C-O	-6.50	1.16	1.24
1	u	20	THR	C-O	-6.49	1.16	1.24
1	H	44	THR	C-O	-6.49	1.16	1.24
1	U	149	TYR	C-O	-6.49	1.16	1.24
1	E	26	PHE	C-O	-6.49	1.16	1.24
1	i	135	GLU	C-O	-6.49	1.16	1.24
1	o	151	ALA	C-O	-6.49	1.16	1.24
1	s	14	GLN	C-O	-6.49	1.16	1.24
1	X	46	ALA	C-O	-6.48	1.16	1.24
1	b	76	SER	C-O	-6.48	1.16	1.24
1	P	31	MET	C-O	-6.48	1.16	1.24
1	m	98	LEU	C-O	-6.48	1.16	1.24
1	o	75	GLY	C-O	-6.48	1.16	1.23
1	R	45	ARG	C-O	-6.47	1.16	1.24
1	S	138	LEU	C-O	-6.47	1.16	1.24
1	C	61	ARG	C-O	-6.47	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	127	GLU	C-O	-6.47	1.16	1.24
1	S	27	LEU	C-O	-6.47	1.16	1.24
1	T	140	LEU	C-O	-6.47	1.16	1.24
1	e	21	ALA	CA-CB	-6.47	1.43	1.53
1	T	34	ASN	C-O	-6.46	1.16	1.24
1	m	85	GLU	C-O	-6.46	1.16	1.24
1	h	100	ARG	C-O	-6.46	1.16	1.24
1	s	32	GLN	C-O	-6.46	1.16	1.24
1	P	42	ALA	C-O	-6.46	1.16	1.24
1	f	42	ALA	C-O	-6.46	1.16	1.24
1	t	26	PHE	C-O	-6.46	1.16	1.24
1	u	33	ASP	C-O	-6.46	1.16	1.24
1	j	91	LEU	C-O	-6.46	1.16	1.24
1	G	137	GLN	C-O	-6.46	1.16	1.24
1	U	125	ALA	CA-CB	-6.45	1.43	1.53
1	G	108	CYS	C-O	-6.45	1.16	1.24
1	I	39	GLU	C-O	-6.45	1.16	1.24
1	t	98	LEU	C-O	-6.45	1.16	1.24
1	n	105	ILE	C-O	-6.45	1.16	1.24
1	o	141	MET	C-O	-6.45	1.16	1.24
1	J	110	GLU	C-O	-6.45	1.16	1.24
1	K	92	ALA	C-O	-6.45	1.16	1.24
1	P	60	ASP	C-O	-6.45	1.16	1.24
1	g	30	LYS	C-O	-6.45	1.16	1.24
1	G	74	ILE	C-O	-6.44	1.17	1.24
1	u	53	ARG	C-O	-6.44	1.16	1.24
1	H	85	GLU	C-O	-6.44	1.16	1.24
1	a	15	LEU	C-O	-6.44	1.16	1.24
1	m	90	ASP	C-O	-6.44	1.16	1.24
1	a	118	VAL	C-O	-6.44	1.16	1.24
1	o	127	GLU	C-O	-6.44	1.16	1.24
1	D	42	ALA	C-O	-6.44	1.16	1.24
1	x	42	ALA	C-O	-6.44	1.16	1.24
1	P	41	ALA	C-O	-6.43	1.16	1.24
1	m	17	SER	C-O	-6.43	1.16	1.24
1	S	88	GLU	C-O	-6.43	1.16	1.24
1	s	156	ARG	C-O	-6.43	1.19	1.25
1	v	86	GLN	C-O	-6.43	1.16	1.24
1	a	20	THR	C-O	-6.43	1.16	1.24
1	v	41	ALA	C-O	-6.43	1.16	1.24
1	c	106	VAL	C-O	-6.43	1.16	1.24
1	A	100	ARG	C-O	-6.42	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	9	ARG	C-O	-6.42	1.16	1.24
1	e	156	ARG	C-O	-6.42	1.19	1.25
1	r	24	GLN	C-O	-6.42	1.16	1.24
1	w	46	ALA	CA-CB	-6.42	1.43	1.53
1	p	105	ILE	C-O	-6.42	1.16	1.24
1	N	86	GLN	C-O	-6.41	1.16	1.24
1	p	63	LEU	C-O	-6.41	1.16	1.24
1	s	123	ILE	C-O	-6.41	1.16	1.24
1	l	68	LEU	C-O	-6.41	1.18	1.24
1	n	21	ALA	CA-CB	-6.41	1.42	1.53
1	J	43	HIS	C-O	-6.41	1.16	1.24
1	e	20	THR	C-O	-6.41	1.16	1.24
1	v	139	GLU	C-O	-6.40	1.16	1.24
1	A	91	LEU	C-O	-6.40	1.16	1.24
1	G	131	ILE	C-O	-6.40	1.16	1.24
1	a	59	THR	C-O	-6.40	1.16	1.24
1	O	32	GLN	C-O	-6.39	1.16	1.24
1	v	100	ARG	C-O	-6.39	1.16	1.24
1	G	150	SER	C-O	-6.39	1.16	1.24
1	L	91	LEU	C-O	-6.39	1.16	1.24
1	D	13	GLU	C-O	-6.38	1.16	1.24
1	W	61	ARG	C-O	-6.38	1.16	1.24
1	a	130	HIS	C-O	-6.38	1.16	1.24
1	o	25	TYR	C-O	-6.38	1.16	1.24
1	p	9	ARG	C-O	-6.38	1.16	1.24
1	w	39	GLU	C-O	-6.38	1.16	1.24
1	Q	69	PRO	C-O	-6.37	1.17	1.23
1	E	117	ALA	CA-CB	-6.37	1.43	1.53
1	J	33	ASP	C-O	-6.37	1.16	1.24
1	O	11	LEU	C-O	-6.37	1.16	1.24
1	s	131	ILE	C-O	-6.37	1.16	1.24
1	I	120	LEU	C-O	-6.37	1.16	1.24
1	W	63	LEU	C-O	-6.37	1.16	1.24
1	o	55	ALA	C-O	-6.37	1.16	1.24
1	D	47	GLU	C-O	-6.36	1.16	1.24
1	R	110	GLU	C-O	-6.36	1.16	1.24
1	L	118	VAL	C-O	-6.36	1.16	1.24
1	W	22	ILE	C-O	-6.36	1.17	1.24
1	e	138	LEU	C-O	-6.36	1.16	1.24
1	u	123	ILE	C-O	-6.36	1.16	1.24
1	M	54	HIS	C-O	-6.36	1.16	1.24
1	g	14	GLN	C-O	-6.36	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	41	ALA	C-O	-6.36	1.16	1.24
1	C	11	LEU	C-O	-6.36	1.16	1.24
1	I	7	VAL	C-O	-6.35	1.17	1.24
1	u	22	ILE	C-O	-6.35	1.17	1.24
1	U	142	ASP	C-O	-6.35	1.16	1.24
1	x	62	ILE	C-O	-6.35	1.17	1.24
1	O	23	ASN	C-O	-6.34	1.16	1.24
1	p	118	VAL	C-O	-6.34	1.16	1.24
1	M	43	HIS	C-O	-6.34	1.16	1.24
1	o	137	GLN	C-O	-6.34	1.16	1.24
1	s	54	HIS	C-O	-6.34	1.16	1.24
1	R	47	GLU	C-O	-6.33	1.16	1.24
1	t	140	LEU	C-O	-6.33	1.16	1.24
1	T	17	SER	C-O	-6.33	1.16	1.24
1	f	103	PRO	C-O	-6.33	1.16	1.24
1	d	129	GLU	C-O	-6.33	1.16	1.24
1	C	27	LEU	C-O	-6.33	1.16	1.24
1	X	47	GLU	C-O	-6.33	1.16	1.24
1	n	15	LEU	C-O	-6.33	1.16	1.24
1	O	101	LEU	C-O	-6.33	1.16	1.24
1	n	111	LYS	C-O	-6.33	1.15	1.24
1	v	133	TYR	C-O	-6.33	1.16	1.24
1	M	105	ILE	C-O	-6.33	1.16	1.24
1	Q	97	VAL	C-O	-6.33	1.17	1.24
1	a	69	PRO	C-O	-6.33	1.16	1.23
1	b	14	GLN	C-O	-6.33	1.16	1.24
1	h	55	ALA	C-O	-6.33	1.16	1.24
1	P	63	LEU	C-O	-6.32	1.16	1.24
1	V	124	VAL	C-O	-6.32	1.16	1.24
1	e	85	GLU	C-O	-6.32	1.16	1.24
1	p	141	MET	C-O	-6.32	1.16	1.24
1	q	97	VAL	C-O	-6.32	1.17	1.24
1	L	138	LEU	C-O	-6.32	1.16	1.24
1	b	58	ILE	C-O	-6.32	1.16	1.24
1	i	132	ASP	C-O	-6.32	1.16	1.24
1	m	113	ASP	C-O	-6.31	1.15	1.23
1	r	115	THR	C-O	-6.31	1.16	1.24
1	D	123	ILE	C-O	-6.31	1.16	1.24
1	Q	39	GLU	C-O	-6.31	1.16	1.24
1	g	73	ARG	C-O	-6.31	1.16	1.23
1	v	69	PRO	C-O	-6.31	1.15	1.23
1	H	53	ARG	C-N	-6.30	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	m	100	ARG	C-O	-6.30	1.16	1.24
1	C	77	LEU	C-O	-6.30	1.16	1.23
1	Q	125	ALA	C-O	-6.30	1.16	1.24
1	W	126	ASP	C-O	-6.30	1.16	1.24
1	w	156	ARG	C-O	-6.30	1.17	1.24
1	C	101	LEU	C-O	-6.30	1.16	1.24
1	x	125	ALA	C-O	-6.30	1.16	1.24
1	L	151	ALA	C-O	-6.30	1.16	1.24
1	M	28	HIS	C-O	-6.30	1.16	1.24
1	R	138	LEU	C-O	-6.30	1.16	1.24
1	P	29	SER	C-O	-6.29	1.16	1.24
1	S	119	LEU	C-O	-6.29	1.16	1.24
1	c	147	GLU	C-O	-6.29	1.16	1.24
1	H	7	VAL	C-O	-6.29	1.17	1.24
1	H	97	VAL	C-O	-6.29	1.17	1.24
1	N	93	ILE	C-O	-6.29	1.16	1.24
1	v	125	ALA	CA-CB	-6.29	1.43	1.53
1	x	109	ARG	C-O	-6.29	1.16	1.24
1	J	146	GLU	C-O	-6.29	1.16	1.24
1	k	15	LEU	C-O	-6.29	1.16	1.24
1	v	47	GLU	C-O	-6.29	1.16	1.24
1	w	62	ILE	C-O	-6.29	1.17	1.24
1	L	38	THR	C-O	-6.29	1.16	1.24
1	B	15	LEU	C-O	-6.28	1.16	1.24
1	I	76	SER	C-O	-6.28	1.16	1.24
1	J	22	ILE	C-O	-6.28	1.17	1.24
1	Q	92	ALA	C-O	-6.28	1.16	1.24
1	R	84	ARG	C-O	-6.28	1.16	1.24
1	f	110	GLU	C-O	-6.28	1.16	1.24
1	T	114	THR	C-O	-6.28	1.16	1.24
1	I	47	GLU	C-O	-6.28	1.16	1.24
1	m	130	HIS	C-O	-6.28	1.16	1.24
1	p	97	VAL	C-O	-6.28	1.16	1.24
1	r	123	ILE	CA-CB	-6.28	1.46	1.54
1	J	56	GLU	C-O	-6.27	1.16	1.24
1	N	108	CYS	C-O	-6.27	1.16	1.24
1	q	59	THR	C-O	-6.27	1.16	1.24
1	H	53	ARG	C-O	-6.27	1.16	1.24
1	d	115	THR	C-O	-6.27	1.16	1.24
1	e	16	THR	C-O	-6.27	1.16	1.24
1	U	88	GLU	C-O	-6.27	1.16	1.24
1	V	133	TYR	C-O	-6.27	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	u	9	ARG	C-O	-6.27	1.16	1.24
1	a	131	ILE	C-O	-6.27	1.17	1.24
1	j	83	LEU	C-O	-6.27	1.16	1.24
1	S	19	LEU	C-O	-6.26	1.16	1.24
1	o	97	VAL	C-O	-6.26	1.17	1.24
1	P	32	GLN	C-O	-6.26	1.16	1.24
1	h	5	PRO	C-O	-6.26	1.16	1.24
1	o	70	ASN	C-O	-6.26	1.16	1.24
1	s	85	GLU	C-O	-6.26	1.16	1.24
1	c	89	ALA	CA-CB	-6.26	1.43	1.53
1	l	64	LEU	C-O	-6.26	1.16	1.24
1	m	97	VAL	C-O	-6.26	1.17	1.24
1	E	31	MET	C-O	-6.26	1.16	1.24
1	w	102	LYS	C-O	-6.26	1.18	1.24
1	C	89	ALA	C-O	-6.26	1.16	1.24
1	q	102	LYS	C-O	-6.26	1.18	1.24
1	d	79	ILE	C-O	-6.25	1.16	1.23
1	p	60	ASP	C-O	-6.25	1.17	1.24
1	G	102	LYS	N-CA	-6.25	1.41	1.46
1	f	107	MET	C-O	-6.25	1.17	1.24
1	v	40	LEU	C-O	-6.25	1.16	1.24
1	B	32	GLN	C-O	-6.25	1.16	1.24
1	x	134	LEU	C-O	-6.25	1.16	1.24
1	l	9	ARG	C-O	-6.25	1.16	1.24
1	U	33	ASP	C-O	-6.24	1.16	1.24
1	R	118	VAL	C-O	-6.24	1.16	1.24
1	A	74	ILE	C-O	-6.24	1.17	1.24
1	o	31	MET	C-O	-6.24	1.16	1.24
1	x	150	SER	C-O	-6.24	1.16	1.24
1	J	38	THR	C-O	-6.23	1.16	1.24
1	P	22	ILE	C-O	-6.23	1.17	1.24
1	S	2	GLN	C-O	-6.23	1.17	1.23
1	T	85	GLU	C-O	-6.23	1.16	1.24
1	o	130	HIS	C-O	-6.23	1.17	1.24
1	C	105	ILE	C-O	-6.23	1.16	1.24
1	U	73	ARG	C-O	-6.23	1.16	1.24
1	b	27	LEU	C-O	-6.23	1.16	1.24
1	G	127	GLU	C-O	-6.23	1.16	1.24
1	T	74	ILE	C-O	-6.23	1.17	1.24
1	r	60	ASP	C-O	-6.23	1.16	1.24
1	X	28	HIS	C-O	-6.23	1.16	1.24
1	O	43	HIS	C-O	-6.22	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	20	THR	C-O	-6.22	1.16	1.24
1	t	76	SER	C-O	-6.22	1.16	1.24
1	f	7	VAL	C-O	-6.22	1.17	1.24
1	t	93	ILE	C-O	-6.22	1.16	1.24
1	b	70	ASN	C-O	-6.22	1.16	1.24
1	o	132	ASP	C-O	-6.22	1.16	1.24
1	x	10	LEU	C-O	-6.22	1.16	1.24
1	T	120	LEU	C-O	-6.22	1.16	1.24
1	g	108	CYS	C-O	-6.22	1.17	1.24
1	B	19	LEU	C-O	-6.22	1.16	1.24
1	G	4	ASP	C-O	-6.22	1.16	1.24
1	V	34	ASN	C-O	-6.22	1.16	1.24
1	f	51	GLU	C-O	-6.22	1.16	1.24
1	u	45	ARG	C-O	-6.22	1.17	1.24
1	Q	32	GLN	C-O	-6.21	1.17	1.24
1	O	119	LEU	C-O	-6.21	1.17	1.24
1	P	102	LYS	C-O	-6.21	1.18	1.24
1	f	8	LEU	C-O	-6.21	1.16	1.24
1	u	46	ALA	C-O	-6.21	1.16	1.24
1	x	40	LEU	C-O	-6.21	1.16	1.24
1	P	50	ASP	C-O	-6.21	1.17	1.24
1	Q	99	ASN	C-O	-6.21	1.16	1.24
1	C	53	ARG	C-O	-6.21	1.16	1.24
1	U	138	LEU	C-O	-6.20	1.16	1.24
1	X	31	MET	C-O	-6.20	1.17	1.24
1	c	116	SER	C-N	6.20	1.41	1.33
1	h	41	ALA	C-O	-6.20	1.16	1.24
1	l	83	LEU	C-O	-6.20	1.17	1.24
1	t	35	TRP	C-O	-6.20	1.16	1.24
1	n	92	ALA	C-O	-6.20	1.16	1.24
1	v	14	GLN	C-O	-6.20	1.16	1.24
1	G	121	GLU	C-O	-6.20	1.16	1.24
1	L	30	LYS	C-O	-6.20	1.16	1.24
1	Q	136	THR	C-O	-6.20	1.16	1.24
1	T	27	LEU	C-O	-6.20	1.16	1.24
1	T	48	SER	C-O	-6.20	1.16	1.24
1	v	132	ASP	C-O	-6.20	1.17	1.24
1	s	8	LEU	C-O	-6.20	1.16	1.24
1	D	141	MET	C-O	-6.19	1.17	1.24
1	L	115	THR	C-O	-6.19	1.17	1.24
1	w	42	ALA	C-O	-6.19	1.16	1.24
1	J	105	ILE	C-O	-6.19	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	42	ALA	C-O	-6.19	1.17	1.24
1	o	42	ALA	C-O	-6.19	1.16	1.24
1	G	116	SER	C-O	-6.19	1.16	1.24
1	K	39	GLU	C-O	-6.19	1.17	1.24
1	p	136	THR	C-O	-6.18	1.16	1.24
1	G	20	THR	C-O	-6.18	1.17	1.24
1	H	41	ALA	C-O	-6.18	1.16	1.24
1	i	139	GLU	C-O	-6.18	1.16	1.24
1	D	134	LEU	C-O	-6.18	1.16	1.24
1	k	117	ALA	CA-CB	-6.18	1.43	1.53
1	G	123	ILE	C-O	-6.17	1.17	1.24
1	e	75	GLY	C-O	-6.17	1.18	1.23
1	x	47	GLU	C-O	-6.17	1.16	1.24
1	B	27	LEU	C-O	-6.17	1.16	1.24
1	D	88	GLU	C-O	-6.17	1.16	1.24
1	F	59	THR	C-O	-6.17	1.17	1.24
1	H	27	LEU	C-O	-6.17	1.17	1.24
1	w	13	GLU	C-O	-6.17	1.17	1.24
1	X	41	ALA	C-O	-6.17	1.17	1.24
1	X	45	ARG	C-O	-6.17	1.17	1.24
1	a	105	ILE	C-O	-6.17	1.16	1.24
1	x	46	ALA	C-O	-6.17	1.17	1.24
1	g	42	ALA	CA-CB	-6.16	1.43	1.53
1	u	32	GLN	C-O	-6.16	1.17	1.24
1	t	13	GLU	C-O	-6.16	1.17	1.24
1	G	99	ASN	C-O	-6.16	1.17	1.24
1	T	135	GLU	C-O	-6.16	1.16	1.24
1	E	149	TYR	C-O	-6.16	1.17	1.24
1	G	21	ALA	C-O	-6.16	1.17	1.24
1	v	57	GLU	C-O	-6.16	1.17	1.24
1	f	135	GLU	C-O	-6.15	1.17	1.24
1	I	89	ALA	C-O	-6.15	1.17	1.24
1	j	154	VAL	C-O	-6.15	1.15	1.24
1	O	136	THR	C-O	-6.15	1.16	1.24
1	b	6	ASP	C-O	-6.15	1.16	1.24
1	D	97	VAL	C-O	-6.15	1.17	1.24
1	X	27	LEU	C-O	-6.15	1.17	1.24
1	m	45	ARG	C-O	-6.15	1.17	1.24
1	m	131	ILE	C-O	-6.15	1.17	1.24
1	s	117	ALA	C-O	-6.15	1.17	1.24
1	u	59	THR	C-O	-6.15	1.17	1.24
1	W	31	MET	C-O	-6.14	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	d	61	ARG	C-O	-6.14	1.17	1.24
1	G	138	LEU	C-O	-6.14	1.17	1.24
1	d	48	SER	C-O	-6.14	1.17	1.24
1	o	87	PHE	C-O	-6.14	1.16	1.24
1	A	41	ALA	C-O	-6.13	1.16	1.24
1	D	117	ALA	C-O	-6.13	1.17	1.24
1	X	12	ASN	C-O	-6.13	1.16	1.24
1	h	69	PRO	C-O	-6.13	1.17	1.23
1	n	44	THR	C-O	-6.13	1.17	1.24
1	W	45	ARG	C-O	-6.13	1.17	1.24
1	c	83	LEU	C-O	-6.13	1.17	1.24
1	h	94	GLU	C-O	-6.13	1.17	1.24
1	B	74	ILE	C-O	-6.12	1.17	1.24
1	T	79	ILE	C-O	-6.12	1.17	1.24
1	o	7	VAL	C-O	-6.12	1.17	1.24
1	x	107	MET	C-O	-6.12	1.17	1.24
1	p	24	GLN	C-O	-6.12	1.17	1.24
1	c	49	PHE	C-O	-6.12	1.17	1.24
1	S	151	ALA	C-O	-6.12	1.17	1.24
1	j	87	PHE	C-O	-6.12	1.17	1.24
1	q	22	ILE	C-O	-6.12	1.17	1.24
1	t	119	LEU	C-O	-6.12	1.17	1.24
1	F	126	ASP	C-O	-6.12	1.17	1.24
1	b	84	ARG	C-O	-6.12	1.17	1.24
1	X	68	LEU	C-O	-6.12	1.17	1.24
1	h	22	ILE	C-O	-6.12	1.17	1.24
1	D	10	LEU	C-O	-6.11	1.17	1.24
1	L	124	VAL	C-O	-6.11	1.17	1.24
1	v	123	ILE	C-O	-6.11	1.16	1.24
1	S	79	ILE	C-O	-6.11	1.17	1.24
1	h	27	LEU	C-O	-6.11	1.17	1.24
1	D	7	VAL	C-O	-6.11	1.17	1.24
1	u	131	ILE	C-O	-6.11	1.17	1.24
1	a	156	ARG	C-O	-6.11	1.20	1.25
1	B	29	SER	C-O	-6.11	1.17	1.24
1	g	39	GLU	C-O	-6.11	1.16	1.24
1	T	128	GLU	C-O	-6.11	1.17	1.24
1	l	115	THR	C-O	-6.11	1.17	1.24
1	W	19	LEU	C-O	-6.10	1.16	1.24
1	s	149	TYR	C-O	-6.10	1.17	1.24
1	I	49	PHE	C-O	-6.10	1.17	1.24
1	h	123	ILE	C-O	-6.10	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	24	GLN	C-N	-6.10	1.25	1.33
1	X	85	GLU	C-O	-6.10	1.17	1.24
1	c	54	HIS	C-O	-6.10	1.16	1.24
1	j	88	GLU	C-O	-6.10	1.17	1.24
1	g	131	ILE	C-O	-6.10	1.17	1.24
1	s	69	PRO	C-O	-6.09	1.16	1.23
1	u	15	LEU	C-O	-6.09	1.17	1.24
1	A	135	GLU	C-O	-6.09	1.17	1.24
1	a	135	GLU	C-O	-6.09	1.17	1.24
1	o	128	GLU	C-O	-6.09	1.17	1.24
1	r	55	ALA	C-O	-6.09	1.17	1.24
1	u	135	GLU	C-O	-6.09	1.17	1.24
1	G	13	GLU	C-O	-6.09	1.17	1.24
1	f	12	ASN	C-O	-6.09	1.16	1.24
1	T	59	THR	C-O	-6.08	1.17	1.24
1	u	63	LEU	C-O	-6.08	1.17	1.24
1	V	9	ARG	C-O	-6.08	1.16	1.24
1	j	40	LEU	C-O	-6.08	1.17	1.24
1	M	46	ALA	C-O	-6.08	1.17	1.24
1	T	132	ASP	C-O	-6.08	1.17	1.24
1	n	116	SER	C-O	-6.08	1.16	1.24
1	p	54	HIS	C-O	-6.08	1.17	1.24
1	D	85	GLU	C-O	-6.07	1.16	1.24
1	M	93	ILE	C-O	-6.07	1.17	1.24
1	m	42	ALA	C-O	-6.07	1.17	1.24
1	r	52	MET	C-O	-6.07	1.17	1.24
1	K	11	LEU	C-O	-6.07	1.17	1.24
1	N	4	ASP	C-O	-6.07	1.15	1.24
1	C	108	CYS	C-O	-6.07	1.17	1.24
1	N	82	THR	C-O	-6.07	1.16	1.23
1	U	135	GLU	C-O	-6.07	1.17	1.24
1	X	125	ALA	C-O	-6.07	1.17	1.24
1	d	12	ASN	C-O	-6.07	1.16	1.24
1	i	59	THR	C-O	-6.07	1.17	1.24
1	k	102	LYS	C-O	-6.07	1.18	1.24
1	o	41	ALA	C-O	-6.07	1.17	1.24
1	u	49	PHE	C-O	-6.07	1.17	1.24
1	B	129	GLU	C-O	-6.07	1.17	1.24
1	d	121	GLU	C-O	-6.07	1.17	1.24
1	k	131	ILE	CA-CB	-6.07	1.46	1.54
1	g	27	LEU	C-O	-6.06	1.17	1.24
1	i	72	GLN	C-O	-6.06	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	87	PHE	C-O	-6.06	1.17	1.24
1	C	46	ALA	CA-CB	-6.06	1.43	1.53
1	L	33	ASP	C-O	-6.05	1.17	1.24
1	M	41	ALA	C-O	-6.05	1.17	1.24
1	i	117	ALA	CA-CB	-6.05	1.44	1.53
1	A	55	ALA	CA-CB	-6.05	1.44	1.53
1	H	42	ALA	C-O	-6.05	1.17	1.24
1	N	14	GLN	C-O	-6.05	1.17	1.24
1	b	147	GLU	C-O	-6.05	1.17	1.24
1	Q	116	SER	C-O	-6.05	1.17	1.24
1	C	132	ASP	C-O	-6.05	1.17	1.24
1	J	47	GLU	C-O	-6.05	1.17	1.24
1	W	131	ILE	C-O	-6.05	1.17	1.24
1	d	29	SER	C-O	-6.05	1.17	1.24
1	j	47	GLU	C-O	-6.05	1.17	1.24
1	l	26	PHE	C-O	-6.05	1.17	1.24
1	u	96	ASP	C-O	-6.05	1.17	1.24
1	U	34	ASN	C-O	-6.04	1.17	1.24
1	b	32	GLN	C-O	-6.04	1.17	1.24
1	q	41	ALA	C-O	-6.04	1.17	1.24
1	c	151	ALA	C-O	-6.04	1.16	1.24
1	L	139	GLU	C-O	-6.04	1.17	1.24
1	t	96	ASP	C-O	-6.04	1.17	1.24
1	F	115	THR	C-O	-6.04	1.17	1.24
1	B	151	ALA	C-O	-6.04	1.16	1.24
1	D	127	GLU	C-O	-6.04	1.17	1.24
1	f	102	LYS	C-O	-6.04	1.18	1.24
1	D	43	HIS	C-O	-6.03	1.17	1.24
1	X	130	HIS	C-O	-6.03	1.17	1.24
1	m	119	LEU	C-O	-6.03	1.17	1.24
1	o	105	ILE	C-O	-6.03	1.17	1.24
1	I	22	ILE	C-O	-6.03	1.17	1.24
1	K	105	ILE	C-O	-6.03	1.17	1.24
1	N	42	ALA	C-O	-6.03	1.17	1.24
1	x	118	VAL	C-O	-6.03	1.17	1.24
1	K	84	ARG	C-O	-6.03	1.17	1.24
1	R	42	ALA	C-O	-6.03	1.17	1.24
1	f	45	ARG	C-O	-6.03	1.17	1.24
1	t	95	TYR	C-O	-6.03	1.16	1.24
1	g	95	TYR	C-O	-6.03	1.17	1.24
1	m	16	THR	C-O	-6.03	1.17	1.24
1	n	69	PRO	C-O	-6.03	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	u	94	GLU	C-O	-6.03	1.17	1.24
1	w	118	VAL	C-O	-6.03	1.17	1.24
1	n	34	ASN	C-O	-6.02	1.17	1.24
1	D	54	HIS	C-O	-6.02	1.17	1.24
1	D	154	VAL	C-O	-6.02	1.16	1.24
1	V	97	VAL	C-O	-6.02	1.17	1.24
1	k	23	ASN	C-O	-6.02	1.17	1.24
1	m	106	VAL	C-O	-6.02	1.17	1.24
1	E	16	THR	C-O	-6.01	1.17	1.24
1	h	96	ASP	C-O	-6.01	1.17	1.24
1	x	74	ILE	C-O	-6.01	1.17	1.23
1	I	23	ASN	C-O	-6.01	1.17	1.24
1	O	108	CYS	C-O	-6.01	1.17	1.24
1	X	142	ASP	C-O	-6.01	1.17	1.24
1	l	41	ALA	CA-CB	-6.01	1.44	1.53
1	V	56	GLU	C-O	-6.01	1.17	1.24
1	J	129	GLU	C-O	-6.01	1.17	1.24
1	Q	103	PRO	C-O	-6.01	1.17	1.24
1	o	38	THR	C-O	-6.01	1.17	1.24
1	P	44	THR	C-O	-6.01	1.17	1.24
1	g	115	THR	C-O	-6.01	1.17	1.24
1	N	13	GLU	C-O	-6.00	1.17	1.24
1	Q	87	PHE	C-O	-6.00	1.17	1.24
1	w	131	ILE	C-O	-6.00	1.17	1.24
1	P	129	GLU	C-O	-6.00	1.17	1.24
1	n	46	ALA	C-O	-6.00	1.17	1.24
1	I	12	ASN	C-O	-6.00	1.17	1.24
1	K	15	LEU	C-O	-6.00	1.17	1.24
1	U	103	PRO	C-O	-6.00	1.17	1.24
1	g	18	GLU	C-O	-6.00	1.17	1.24
1	w	63	LEU	C-O	-6.00	1.17	1.24
1	h	47	GLU	C-O	-5.99	1.17	1.24
1	x	138	LEU	C-O	-5.99	1.17	1.24
1	R	56	GLU	C-O	-5.99	1.17	1.24
1	D	127	GLU	C-N	-5.99	1.26	1.33
1	P	115	THR	C-O	-5.99	1.17	1.24
1	S	135	GLU	C-O	-5.99	1.17	1.24
1	T	146	GLU	C-O	-5.99	1.17	1.24
1	G	33	ASP	C-O	-5.99	1.17	1.24
1	J	24	GLN	C-O	-5.99	1.17	1.24
1	p	64	LEU	C-O	-5.99	1.17	1.24
1	E	22	ILE	C-O	-5.98	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	46	ALA	C-O	-5.98	1.17	1.24
1	x	144	LEU	C-O	-5.98	1.16	1.24
1	m	136	THR	C-O	-5.98	1.17	1.24
1	m	141	MET	C-O	-5.98	1.17	1.24
1	K	46	ALA	C-O	-5.98	1.17	1.24
1	q	19	LEU	C-O	-5.98	1.17	1.24
1	v	121	GLU	C-O	-5.98	1.17	1.24
1	w	151	ALA	C-O	-5.98	1.16	1.24
1	Q	57	GLU	C-O	-5.97	1.17	1.24
1	g	106	VAL	C-O	-5.97	1.17	1.24
1	u	139	GLU	C-O	-5.97	1.17	1.24
1	N	17	SER	C-O	-5.97	1.17	1.24
1	q	109	ARG	C-O	-5.97	1.16	1.24
1	E	43	HIS	C-O	-5.97	1.17	1.24
1	N	151	ALA	C-O	-5.97	1.16	1.24
1	o	92	ALA	C-O	-5.97	1.17	1.24
1	v	120	LEU	C-O	-5.97	1.16	1.24
1	K	54	HIS	C-O	-5.97	1.17	1.24
1	O	64	LEU	C-O	-5.97	1.17	1.24
1	T	129	GLU	C-O	-5.96	1.17	1.24
1	a	85	GLU	C-O	-5.96	1.17	1.24
1	q	25	TYR	C-O	-5.96	1.17	1.24
1	a	150	SER	C-O	-5.96	1.16	1.24
1	o	65	LEU	C-O	-5.96	1.16	1.24
1	N	98	LEU	C-O	-5.96	1.16	1.24
1	U	150	SER	C-O	-5.96	1.16	1.24
1	I	133	TYR	C-O	-5.96	1.17	1.24
1	m	138	LEU	C-O	-5.96	1.17	1.24
1	S	9	ARG	C-O	-5.96	1.17	1.24
1	M	92	ALA	C-O	-5.95	1.17	1.24
1	U	114	THR	C-O	-5.95	1.17	1.24
1	g	23	ASN	C-O	-5.95	1.17	1.24
1	K	107	MET	C-O	-5.95	1.17	1.24
1	L	133	TYR	C-O	-5.95	1.17	1.24
1	B	99	ASN	C-O	-5.95	1.17	1.24
1	M	143	LYS	C-O	-5.95	1.17	1.24
1	b	131	ILE	C-O	-5.95	1.17	1.24
1	n	42	ALA	C-O	-5.95	1.17	1.24
1	t	117	ALA	C-O	-5.95	1.17	1.24
1	D	41	ALA	CA-CB	-5.95	1.44	1.53
1	u	13	GLU	C-O	-5.95	1.17	1.24
1	H	110	GLU	C-O	-5.95	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	49	PHE	C-O	-5.95	1.17	1.24
1	l	23	ASN	C-O	-5.94	1.17	1.24
1	T	53	ARG	C-O	-5.94	1.17	1.24
1	n	27	LEU	C-O	-5.94	1.17	1.24
1	p	51	GLU	C-O	-5.94	1.16	1.24
1	I	141	MET	C-O	-5.94	1.17	1.24
1	V	21	ALA	C-O	-5.94	1.17	1.24
1	f	50	ASP	C-O	-5.94	1.17	1.24
1	i	43	HIS	C-O	-5.94	1.17	1.24
1	J	149	TYR	C-O	-5.94	1.17	1.24
1	d	42	ALA	CA-CB	-5.94	1.43	1.53
1	x	70	ASN	C-O	-5.94	1.16	1.23
1	o	24	GLN	C-O	-5.94	1.17	1.24
1	S	28	HIS	C-O	-5.93	1.17	1.24
1	W	107	MET	C-O	-5.93	1.17	1.24
1	j	123	ILE	C-O	-5.93	1.17	1.24
1	J	92	ALA	C-O	-5.93	1.17	1.24
1	v	28	HIS	C-O	-5.93	1.17	1.24
1	G	45	ARG	C-O	-5.93	1.17	1.24
1	R	59	THR	C-O	-5.93	1.17	1.24
1	S	72	GLN	C-O	-5.93	1.17	1.24
1	g	13	GLU	C-O	-5.93	1.17	1.24
1	v	17	SER	C-O	-5.93	1.17	1.24
1	G	119	LEU	C-O	-5.93	1.17	1.24
1	S	106	VAL	C-O	-5.93	1.17	1.24
1	j	146	GLU	C-O	-5.93	1.17	1.24
1	H	54	HIS	C-O	-5.92	1.17	1.24
1	I	131	ILE	C-O	-5.92	1.17	1.24
1	v	24	GLN	C-O	-5.92	1.17	1.24
1	A	133	TYR	C-O	-5.92	1.17	1.24
1	L	116	SER	C-O	-5.92	1.17	1.24
1	s	142	ASP	C-O	-5.92	1.17	1.24
1	a	95	TYR	C-O	-5.92	1.16	1.24
1	a	129	GLU	C-O	-5.92	1.17	1.24
1	o	142	ASP	C-O	-5.92	1.16	1.24
1	B	26	PHE	C-O	-5.92	1.17	1.24
1	P	108	CYS	C-O	-5.92	1.17	1.24
1	T	142	ASP	C-O	-5.92	1.17	1.24
1	n	143	LYS	C-O	-5.92	1.17	1.24
1	k	111	LYS	C-O	-5.92	1.15	1.24
1	Q	145	GLY	C-O	-5.91	1.17	1.24
1	S	94	GLU	C-N	-5.91	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	156	ARG	C-O	-5.91	1.19	1.25
1	b	7	VAL	C-O	-5.91	1.17	1.24
1	m	79	ILE	C-O	-5.91	1.17	1.24
1	Q	129	GLU	C-O	-5.91	1.17	1.24
1	S	86	GLN	C-O	-5.91	1.17	1.24
1	b	124	VAL	C-O	-5.91	1.17	1.24
1	A	64	LEU	C-O	-5.91	1.16	1.24
1	D	146	GLU	C-O	-5.91	1.17	1.24
1	M	53	ARG	C-O	-5.91	1.17	1.24
1	Q	149	TYR	C-O	-5.91	1.17	1.24
1	i	25	TYR	C-O	-5.91	1.17	1.24
1	a	25	TYR	C-O	-5.91	1.17	1.24
1	d	24	GLN	C-O	-5.91	1.17	1.24
1	V	69	PRO	C-O	-5.90	1.17	1.23
1	U	94	GLU	C-O	-5.90	1.17	1.24
1	l	27	LEU	C-O	-5.90	1.17	1.24
1	H	130	HIS	C-O	-5.90	1.17	1.24
1	i	46	ALA	CA-CB	-5.90	1.44	1.53
1	w	127	GLU	C-O	-5.90	1.17	1.24
1	H	40	LEU	C-O	-5.90	1.17	1.24
1	V	114	THR	C-O	-5.90	1.17	1.24
1	W	27	LEU	C-O	-5.90	1.17	1.24
1	X	14	GLN	C-O	-5.90	1.17	1.24
1	c	85	GLU	C-O	-5.90	1.17	1.24
1	C	150	SER	C-O	-5.89	1.17	1.24
1	F	105	ILE	C-O	-5.89	1.17	1.24
1	G	96	ASP	C-O	-5.89	1.17	1.24
1	K	78	ARG	C-O	-5.89	1.16	1.23
1	T	31	MET	C-O	-5.89	1.17	1.24
1	g	4	ASP	C-O	-5.89	1.16	1.24
1	j	98	LEU	C-O	-5.89	1.17	1.24
1	D	79	ILE	C-O	-5.89	1.17	1.24
1	a	7	VAL	C-O	-5.89	1.17	1.24
1	j	121	GLU	C-O	-5.89	1.17	1.24
1	S	26	PHE	C-O	-5.89	1.17	1.24
1	U	117	ALA	C-O	-5.89	1.17	1.24
1	W	111	LYS	C-O	-5.89	1.16	1.24
1	v	108	CYS	C-O	-5.89	1.17	1.24
1	T	35	TRP	C-O	-5.89	1.16	1.24
1	j	147	GLU	C-O	-5.89	1.17	1.24
1	q	143	LYS	C-O	-5.89	1.17	1.24
1	w	116	SER	C-O	-5.89	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	w	128	GLU	C-O	-5.89	1.17	1.24
1	C	83	LEU	C-O	-5.88	1.17	1.24
1	F	41	ALA	CA-CB	-5.88	1.44	1.53
1	S	18	GLU	C-O	-5.88	1.17	1.24
1	p	148	LEU	C-O	-5.88	1.17	1.24
1	v	114	THR	C-O	-5.88	1.17	1.24
1	H	134	LEU	C-O	-5.88	1.17	1.24
1	J	13	GLU	C-O	-5.88	1.17	1.24
1	S	33	ASP	C-O	-5.88	1.17	1.24
1	l	89	ALA	C-O	-5.88	1.17	1.24
1	U	58	ILE	C-O	-5.88	1.17	1.24
1	K	83	LEU	C-O	-5.88	1.17	1.24
1	l	118	VAL	C-O	-5.88	1.17	1.24
1	H	22	ILE	C-O	-5.88	1.17	1.24
1	N	149	TYR	C-O	-5.88	1.17	1.24
1	i	99	ASN	C-O	-5.88	1.17	1.24
1	m	126	ASP	C-O	-5.87	1.17	1.24
1	x	23	ASN	C-O	-5.87	1.17	1.24
1	o	83	LEU	C-O	-5.87	1.17	1.24
1	u	61	ARG	C-O	-5.87	1.17	1.24
1	U	56	GLU	C-O	-5.87	1.17	1.24
1	g	56	GLU	C-O	-5.87	1.17	1.24
1	q	32	GLN	C-O	-5.87	1.17	1.24
1	N	114	THR	C-O	-5.87	1.17	1.24
1	L	12	ASN	C-O	-5.86	1.17	1.24
1	G	15	LEU	C-O	-5.86	1.17	1.24
1	N	135	GLU	C-O	-5.86	1.17	1.24
1	R	60	ASP	C-O	-5.86	1.17	1.24
1	I	32	GLN	C-O	-5.86	1.17	1.24
1	S	60	ASP	C-O	-5.86	1.17	1.24
1	f	62	ILE	C-O	-5.86	1.17	1.24
1	p	75	GLY	C-O	-5.86	1.17	1.23
1	p	79	ILE	C-O	-5.86	1.17	1.24
1	v	142	ASP	C-O	-5.86	1.17	1.24
1	Q	50	ASP	C-O	-5.86	1.17	1.24
1	G	134	LEU	C-O	-5.86	1.17	1.24
1	l	135	GLU	C-O	-5.86	1.17	1.24
1	m	127	GLU	C-O	-5.86	1.17	1.24
1	F	100	ARG	C-O	-5.86	1.17	1.24
1	K	12	ASN	C-O	-5.86	1.17	1.24
1	w	25	TYR	C-N	-5.86	1.26	1.33
1	H	32	GLN	C-O	-5.85	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	2	GLN	C-O	-5.85	1.17	1.24
1	W	26	PHE	C-O	-5.85	1.17	1.24
1	d	139	GLU	C-O	-5.85	1.17	1.24
1	W	112	GLN	C-O	-5.85	1.16	1.23
1	a	117	ALA	C-O	-5.85	1.17	1.24
1	h	39	GLU	C-O	-5.85	1.17	1.24
1	j	151	ALA	C-O	-5.85	1.16	1.24
1	v	64	LEU	C-O	-5.85	1.17	1.24
1	v	19	LEU	C-O	-5.84	1.17	1.24
1	A	127	GLU	C-O	-5.84	1.17	1.24
1	E	143	LYS	C-O	-5.84	1.17	1.24
1	d	141	MET	C-O	-5.84	1.17	1.24
1	v	118	VAL	C-O	-5.84	1.17	1.24
1	F	41	ALA	C-O	-5.84	1.17	1.24
1	V	64	LEU	C-O	-5.84	1.17	1.24
1	s	88	GLU	C-O	-5.84	1.17	1.24
1	i	8	LEU	C-O	-5.83	1.17	1.24
1	i	42	ALA	C-O	-5.83	1.17	1.24
1	G	141	MET	C-O	-5.83	1.17	1.24
1	T	57	GLU	C-O	-5.83	1.17	1.24
1	O	137	GLN	C-O	-5.83	1.17	1.24
1	j	119	LEU	C-O	-5.83	1.17	1.24
1	H	73	ARG	C-O	-5.83	1.16	1.24
1	T	103	PRO	C-O	-5.83	1.17	1.24
1	W	13	GLU	C-O	-5.83	1.17	1.24
1	D	32	GLN	C-O	-5.83	1.17	1.24
1	M	126	ASP	C-O	-5.83	1.17	1.24
1	b	110	GLU	C-O	-5.83	1.17	1.24
1	d	87	PHE	C-O	-5.82	1.17	1.24
1	n	118	VAL	C-O	-5.82	1.17	1.24
1	x	121	GLU	C-O	-5.82	1.17	1.24
1	A	38	THR	C-O	-5.82	1.17	1.24
1	I	68	LEU	C-O	-5.82	1.17	1.24
1	T	91	LEU	C-O	-5.82	1.17	1.24
1	w	34	ASN	C-O	-5.82	1.16	1.24
1	I	138	LEU	C-O	-5.82	1.17	1.24
1	b	25	TYR	C-O	-5.82	1.17	1.24
1	D	76	SER	C-O	-5.82	1.16	1.24
1	J	136	THR	C-O	-5.82	1.17	1.24
1	p	108	CYS	C-O	-5.82	1.17	1.24
1	w	74	ILE	C-O	-5.82	1.18	1.24
1	C	58	ILE	C-O	-5.81	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	s	28	HIS	C-O	-5.81	1.17	1.24
1	q	151	ALA	CA-CB	-5.81	1.43	1.53
1	n	40	LEU	C-O	-5.81	1.16	1.24
1	p	46	ALA	CA-CB	-5.81	1.44	1.53
1	G	79	ILE	C-O	-5.81	1.17	1.24
1	u	41	ALA	C-O	-5.81	1.17	1.24
1	l	11	LEU	C-O	-5.80	1.17	1.24
1	p	58	ILE	C-O	-5.80	1.17	1.24
1	e	31	MET	C-O	-5.80	1.17	1.24
1	f	56	GLU	C-O	-5.80	1.17	1.24
1	F	103	PRO	C-O	-5.80	1.16	1.24
1	n	86	GLN	C-O	-5.80	1.17	1.24
1	T	43	HIS	C-O	-5.80	1.17	1.24
1	h	108	CYS	C-O	-5.80	1.17	1.24
1	j	31	MET	C-O	-5.80	1.17	1.24
1	m	27	LEU	C-O	-5.79	1.17	1.24
1	o	9	ARG	C-O	-5.79	1.17	1.24
1	J	63	LEU	C-O	-5.79	1.17	1.24
1	a	39	GLU	C-O	-5.79	1.17	1.24
1	d	123	ILE	C-O	-5.79	1.17	1.24
1	F	114	THR	C-O	-5.79	1.17	1.24
1	T	121	GLU	C-O	-5.79	1.17	1.24
1	U	98	LEU	C-O	-5.79	1.17	1.24
1	A	40	LEU	C-O	-5.79	1.17	1.24
1	L	21	ALA	CA-CB	-5.79	1.44	1.53
1	a	101	LEU	C-O	-5.79	1.17	1.24
1	m	121	GLU	C-O	-5.79	1.17	1.24
1	B	85	GLU	C-O	-5.79	1.17	1.24
1	K	106	VAL	C-O	-5.79	1.17	1.24
1	R	43	HIS	C-O	-5.79	1.17	1.24
1	b	115	THR	C-O	-5.79	1.17	1.24
1	k	82	THR	C-O	-5.79	1.16	1.23
1	n	123	ILE	C-O	-5.78	1.17	1.24
1	w	5	PRO	C-O	-5.78	1.17	1.24
1	G	10	LEU	C-O	-5.78	1.17	1.24
1	L	124	VAL	CA-CB	5.78	1.61	1.54
1	X	78	ARG	C-O	-5.78	1.17	1.24
1	f	63	LEU	C-O	-5.78	1.16	1.24
1	v	109	ARG	C-O	-5.78	1.17	1.24
1	h	131	ILE	C-O	-5.78	1.17	1.24
1	x	30	LYS	C-O	-5.78	1.17	1.24
1	J	107	MET	C-O	-5.78	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	86	GLN	C-O	-5.78	1.17	1.24
1	X	123	ILE	C-O	-5.78	1.17	1.24
1	g	11	LEU	C-O	-5.78	1.17	1.24
1	b	108	CYS	C-O	-5.77	1.17	1.24
1	f	22	ILE	C-O	-5.77	1.17	1.24
1	r	53	ARG	C-O	-5.77	1.17	1.24
1	F	93	ILE	C-O	-5.77	1.17	1.24
1	N	138	LEU	C-O	-5.77	1.17	1.24
1	n	32	GLN	C-O	-5.77	1.17	1.24
1	A	98	LEU	C-O	-5.77	1.17	1.24
1	c	118	VAL	C-O	-5.77	1.17	1.24
1	x	92	ALA	C-O	-5.77	1.17	1.24
1	T	13	GLU	C-O	-5.77	1.17	1.24
1	U	10	LEU	C-O	-5.77	1.17	1.24
1	V	60	ASP	C-O	-5.77	1.17	1.24
1	x	130	HIS	C-O	-5.77	1.17	1.24
1	F	64	LEU	C-O	-5.76	1.17	1.24
1	U	15	LEU	C-O	-5.76	1.17	1.24
1	u	34	ASN	C-O	-5.76	1.17	1.24
1	B	25	TYR	C-O	-5.76	1.17	1.24
1	R	107	MET	C-O	-5.76	1.17	1.24
1	T	9	ARG	C-O	-5.76	1.17	1.24
1	C	135	GLU	C-O	-5.76	1.17	1.24
1	U	134	LEU	C-O	-5.76	1.17	1.24
1	C	73	ARG	C-O	-5.76	1.16	1.23
1	a	2	GLN	C-O	-5.76	1.17	1.23
1	h	6	ASP	C-O	-5.76	1.17	1.24
1	b	91	LEU	C-O	-5.76	1.17	1.24
1	M	17	SER	C-O	-5.75	1.17	1.24
1	N	106	VAL	C-O	-5.75	1.17	1.24
1	V	40	LEU	C-O	-5.75	1.17	1.24
1	j	24	GLN	C-O	-5.75	1.17	1.24
1	V	151	ALA	CA-CB	-5.75	1.43	1.53
1	W	128	GLU	C-O	-5.75	1.17	1.24
1	l	25	TYR	C-O	-5.75	1.17	1.24
1	A	112	GLN	C-O	-5.75	1.16	1.23
1	L	54	HIS	C-O	-5.75	1.17	1.24
1	u	42	ALA	C-O	-5.75	1.17	1.24
1	m	37	PHE	C-O	-5.75	1.16	1.23
1	I	27	LEU	C-O	-5.75	1.17	1.24
1	S	69	PRO	C-O	-5.75	1.17	1.23
1	t	150	SER	C-O	-5.75	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	141	MET	C-O	-5.75	1.17	1.24
1	N	61	ARG	C-O	-5.74	1.17	1.24
1	n	39	GLU	C-O	-5.74	1.17	1.24
1	P	25	TYR	C-O	-5.74	1.17	1.24
1	S	122	LYS	C-O	-5.74	1.17	1.24
1	f	60	ASP	C-O	-5.74	1.17	1.24
1	F	19	LEU	C-O	-5.74	1.17	1.24
1	d	147	GLU	C-O	-5.74	1.17	1.24
1	f	54	HIS	C-O	-5.74	1.17	1.24
1	U	139	GLU	C-O	-5.74	1.17	1.24
1	N	32	GLN	C-O	-5.74	1.17	1.24
1	a	64	LEU	C-O	-5.74	1.17	1.24
1	n	74	ILE	C-O	-5.74	1.18	1.24
1	t	51	GLU	C-O	-5.74	1.17	1.24
1	u	101	LEU	C-O	-5.73	1.17	1.24
1	A	116	SER	C-O	-5.73	1.17	1.24
1	U	7	VAL	C-O	-5.73	1.17	1.24
1	W	6	ASP	C-O	-5.73	1.17	1.24
1	n	91	LEU	C-O	-5.73	1.17	1.24
1	U	126	ASP	C-O	-5.73	1.17	1.24
1	i	22	ILE	C-O	-5.73	1.17	1.24
1	B	28	HIS	C-O	-5.73	1.17	1.24
1	e	70	ASN	CG-ND2	-5.73	1.21	1.33
1	n	147	GLU	C-O	-5.73	1.17	1.24
1	N	33	ASP	C-O	-5.73	1.17	1.24
1	P	64	LEU	C-O	-5.73	1.17	1.24
1	l	123	ILE	C-O	-5.73	1.17	1.24
1	D	139	GLU	C-O	-5.72	1.17	1.24
1	W	46	ALA	C-O	-5.72	1.17	1.24
1	j	144	LEU	C-O	-5.72	1.16	1.24
1	s	7	VAL	C-O	-5.72	1.17	1.24
1	K	123	ILE	C-O	-5.72	1.17	1.24
1	B	156	ARG	C-O	-5.72	1.19	1.25
1	T	68	LEU	C-O	-5.72	1.18	1.24
1	s	94	GLU	C-O	-5.72	1.17	1.24
1	o	60	ASP	C-O	-5.72	1.17	1.24
1	N	129	GLU	C-O	-5.72	1.17	1.24
1	Q	49	PHE	C-O	-5.72	1.17	1.24
1	s	89	ALA	C-O	-5.72	1.17	1.24
1	A	13	GLU	C-O	-5.71	1.17	1.24
1	o	109	ARG	C-O	-5.71	1.16	1.24
1	N	43	HIS	C-O	-5.71	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	g	114	THR	C-O	-5.71	1.17	1.24
1	D	102	LYS	C-O	-5.71	1.19	1.24
1	w	138	LEU	C-O	-5.71	1.17	1.24
1	T	139	GLU	C-O	-5.71	1.17	1.24
1	g	76	SER	C-O	-5.71	1.17	1.24
1	t	42	ALA	CA-CB	-5.71	1.44	1.53
1	C	136	THR	C-O	-5.71	1.17	1.24
1	X	24	GLN	C-O	-5.71	1.17	1.24
1	b	138	LEU	C-O	-5.71	1.17	1.24
1	e	151	ALA	CA-CB	-5.71	1.44	1.53
1	f	123	ILE	N-CA	-5.71	1.39	1.46
1	J	41	ALA	C-O	-5.71	1.17	1.24
1	b	49	PHE	C-O	-5.71	1.17	1.24
1	C	93	ILE	C-O	-5.70	1.17	1.24
1	O	104	GLY	C-O	-5.70	1.17	1.23
1	T	118	VAL	C-O	-5.70	1.17	1.24
1	d	127	GLU	C-O	-5.70	1.17	1.24
1	d	150	SER	C-O	-5.70	1.17	1.24
1	m	10	LEU	C-O	-5.70	1.17	1.24
1	x	147	GLU	C-O	-5.70	1.17	1.24
1	o	49	PHE	C-O	-5.70	1.17	1.24
1	S	123	ILE	C-O	-5.70	1.17	1.24
1	b	156	ARG	C-O	-5.70	1.18	1.24
1	v	7	VAL	C-O	-5.70	1.17	1.24
1	W	82	THR	C-O	-5.70	1.16	1.23
1	f	69	PRO	C-O	-5.70	1.17	1.23
1	o	72	GLN	C-O	-5.70	1.16	1.24
1	t	156	ARG	C-O	-5.70	1.18	1.24
1	v	12	ASN	C-O	-5.70	1.17	1.24
1	O	41	ALA	C-O	-5.69	1.17	1.24
1	Q	7	VAL	C-O	-5.69	1.17	1.24
1	Q	79	ILE	C-O	-5.69	1.17	1.24
1	p	101	LEU	C-O	-5.69	1.17	1.24
1	T	29	SER	C-O	-5.69	1.17	1.24
1	u	145	GLY	C-O	-5.69	1.16	1.23
1	L	23	ASN	C-O	-5.69	1.17	1.24
1	Q	110	GLU	C-O	-5.69	1.17	1.24
1	a	139	GLU	C-O	-5.69	1.17	1.24
1	M	90	ASP	C-O	-5.69	1.17	1.24
1	E	32	GLN	C-O	-5.68	1.17	1.24
1	U	61	ARG	C-O	-5.68	1.17	1.24
1	n	102	LYS	C-O	-5.68	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	56	GLU	C-O	-5.68	1.17	1.24
1	m	29	SER	C-O	-5.68	1.17	1.24
1	x	139	GLU	C-O	-5.68	1.17	1.24
1	a	137	GLN	C-O	-5.67	1.17	1.24
1	o	89	ALA	C-O	-5.67	1.17	1.24
1	p	29	SER	C-O	-5.67	1.17	1.24
1	B	128	GLU	C-O	-5.67	1.17	1.24
1	e	131	ILE	C-O	-5.67	1.17	1.24
1	v	149	TYR	C-O	-5.67	1.17	1.24
1	X	49	PHE	C-O	-5.67	1.17	1.24
1	b	89	ALA	C-O	-5.67	1.17	1.24
1	i	122	LYS	C-O	-5.67	1.17	1.24
1	o	68	LEU	C-O	-5.67	1.19	1.25
1	r	92	ALA	CA-CB	-5.67	1.44	1.53
1	N	10	LEU	C-O	-5.67	1.17	1.24
1	U	51	GLU	C-O	-5.67	1.17	1.24
1	f	122	LYS	C-O	-5.67	1.17	1.24
1	a	106	VAL	C-O	-5.66	1.17	1.24
1	s	135	GLU	C-O	-5.66	1.17	1.24
1	U	63	LEU	C-O	-5.66	1.17	1.24
1	W	74	ILE	C-O	-5.66	1.18	1.24
1	k	25	TYR	C-O	-5.66	1.17	1.24
1	t	21	ALA	CA-CB	-5.66	1.44	1.53
1	V	74	ILE	C-O	-5.66	1.18	1.24
1	j	7	VAL	C-O	-5.66	1.17	1.24
1	o	136	THR	C-O	-5.66	1.17	1.24
1	v	117	ALA	CA-CB	-5.66	1.44	1.53
1	B	108	CYS	C-O	-5.66	1.17	1.24
1	s	10	LEU	C-O	-5.66	1.17	1.24
1	H	15	LEU	C-O	-5.66	1.17	1.24
1	S	114	THR	C-O	-5.66	1.17	1.24
1	m	39	GLU	C-O	-5.66	1.17	1.24
1	n	127	GLU	C-O	-5.66	1.17	1.24
1	A	23	ASN	C-O	-5.65	1.17	1.24
1	P	97	VAL	C-O	-5.65	1.17	1.24
1	H	71	TYR	C-O	-5.65	1.16	1.24
1	S	21	ALA	CA-CB	-5.65	1.44	1.53
1	l	31	MET	C-O	-5.65	1.17	1.24
1	r	126	ASP	C-O	-5.65	1.17	1.24
1	u	50	ASP	C-O	-5.65	1.17	1.24
1	e	97	VAL	C-O	-5.65	1.17	1.24
1	h	59	THR	C-O	-5.65	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	o	121	GLU	C-O	-5.65	1.17	1.24
1	o	150	SER	C-O	-5.65	1.17	1.24
1	D	28	HIS	C-O	-5.65	1.17	1.24
1	B	117	ALA	C-O	-5.65	1.17	1.24
1	C	147	GLU	C-O	-5.65	1.17	1.24
1	g	123	ILE	C-O	-5.65	1.17	1.24
1	W	134	LEU	C-O	-5.65	1.17	1.24
1	a	27	LEU	C-O	-5.65	1.17	1.24
1	B	102	LYS	C-O	-5.64	1.19	1.24
1	u	88	GLU	C-O	-5.64	1.17	1.24
1	G	76	SER	C-O	-5.64	1.17	1.24
1	n	45	ARG	C-O	-5.64	1.17	1.24
1	u	142	ASP	C-O	-5.64	1.17	1.24
1	q	112	GLN	C-O	-5.64	1.15	1.23
1	u	80	GLY	C-O	-5.64	1.15	1.23
1	v	89	ALA	C-O	-5.64	1.17	1.24
1	O	91	LEU	C-O	-5.64	1.17	1.24
1	g	143	LYS	C-O	-5.64	1.17	1.24
1	E	8	LEU	C-O	-5.64	1.17	1.24
1	I	28	HIS	C-O	-5.64	1.17	1.24
1	f	37	PHE	C-O	-5.64	1.14	1.23
1	o	118	VAL	C-O	-5.64	1.17	1.24
1	D	15	LEU	C-O	-5.63	1.17	1.24
1	a	138	LEU	C-O	-5.63	1.17	1.24
1	g	126	ASP	C-O	-5.63	1.17	1.24
1	t	151	ALA	C-O	-5.63	1.16	1.24
1	P	59	THR	C-O	-5.63	1.17	1.24
1	B	14	GLN	C-O	-5.63	1.17	1.24
1	J	68	LEU	C-O	-5.63	1.18	1.24
1	o	108	CYS	C-O	-5.63	1.17	1.24
1	u	19	LEU	C-O	-5.63	1.17	1.24
1	u	48	SER	C-O	-5.63	1.17	1.24
1	O	151	ALA	C-O	-5.63	1.16	1.24
1	U	116	SER	C-O	-5.63	1.17	1.24
1	V	110	GLU	C-O	-5.63	1.17	1.24
1	S	108	CYS	C-O	-5.63	1.17	1.24
1	U	38	THR	C-O	-5.63	1.17	1.24
1	r	26	PHE	C-O	-5.63	1.17	1.24
1	B	55	ALA	N-CA	-5.63	1.39	1.46
1	U	140	LEU	C-O	-5.62	1.17	1.24
1	e	136	THR	C-O	-5.62	1.17	1.24
1	I	8	LEU	C-O	-5.62	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	58	ILE	C-O	-5.62	1.17	1.24
1	a	31	MET	C-O	-5.62	1.17	1.24
1	C	7	VAL	C-O	-5.62	1.17	1.24
1	j	105	ILE	C-O	-5.62	1.17	1.24
1	i	23	ASN	C-O	-5.62	1.17	1.24
1	k	14	GLN	C-O	-5.62	1.17	1.24
1	N	64	LEU	C-O	-5.62	1.17	1.24
1	C	86	GLN	C-O	-5.62	1.17	1.24
1	G	139	GLU	C-O	-5.62	1.17	1.24
1	H	140	LEU	C-O	-5.62	1.17	1.24
1	N	87	PHE	C-O	-5.62	1.17	1.24
1	w	33	ASP	C-O	-5.62	1.17	1.24
1	J	40	LEU	C-O	-5.61	1.17	1.24
1	V	42	ALA	C-O	-5.61	1.17	1.24
1	B	93	ILE	C-O	-5.61	1.17	1.24
1	I	148	LEU	C-O	-5.61	1.17	1.24
1	d	84	ARG	C-O	-5.61	1.17	1.24
1	W	33	ASP	C-O	-5.61	1.17	1.24
1	F	39	GLU	C-O	-5.61	1.17	1.24
1	q	100	ARG	C-O	-5.61	1.17	1.24
1	C	44	THR	C-O	-5.60	1.17	1.24
1	X	136	THR	C-O	-5.60	1.17	1.24
1	C	106	VAL	C-O	-5.60	1.17	1.24
1	s	150	SER	C-O	-5.60	1.17	1.24
1	f	96	ASP	C-O	-5.60	1.17	1.24
1	B	42	ALA	C-O	-5.60	1.17	1.24
1	G	56	GLU	C-O	-5.60	1.17	1.24
1	l	76	SER	C-O	-5.60	1.17	1.24
1	X	99	ASN	C-O	-5.59	1.17	1.24
1	h	101	LEU	C-O	-5.59	1.17	1.24
1	t	94	GLU	C-O	-5.59	1.17	1.24
1	u	11	LEU	C-O	-5.59	1.17	1.24
1	O	33	ASP	C-O	-5.59	1.17	1.24
1	O	62	ILE	C-O	-5.59	1.17	1.24
1	i	109	ARG	C-O	-5.59	1.17	1.24
1	x	51	GLU	C-O	-5.59	1.17	1.24
1	N	89	ALA	C-O	-5.59	1.17	1.24
1	P	87	PHE	C-O	-5.59	1.17	1.24
1	d	136	THR	C-O	-5.59	1.17	1.24
1	v	103	PRO	C-O	-5.59	1.17	1.24
1	C	49	PHE	C-O	-5.59	1.17	1.24
1	O	19	LEU	C-O	-5.59	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	129	GLU	C-O	-5.59	1.17	1.24
1	I	48	SER	C-O	-5.59	1.17	1.24
1	P	10	LEU	C-O	-5.59	1.17	1.24
1	l	109	ARG	C-O	-5.59	1.17	1.24
1	B	64	LEU	C-O	-5.58	1.17	1.24
1	L	18	GLU	C-O	-5.58	1.17	1.24
1	U	47	GLU	C-O	-5.58	1.17	1.24
1	j	100	ARG	C-O	-5.58	1.17	1.24
1	m	53	ARG	C-O	-5.58	1.17	1.24
1	V	140	LEU	C-O	-5.58	1.17	1.24
1	w	68	LEU	C-O	-5.58	1.20	1.25
1	l	46	ALA	CA-CB	-5.58	1.44	1.53
1	r	137	GLN	C-O	-5.58	1.17	1.24
1	Q	96	ASP	C-O	-5.58	1.17	1.24
1	D	74	ILE	C-O	-5.58	1.18	1.24
1	R	7	VAL	C-O	-5.58	1.17	1.24
1	m	107	MET	C-O	-5.58	1.17	1.24
1	p	41	ALA	C-O	-5.58	1.17	1.24
1	Q	23	ASN	C-O	-5.58	1.17	1.24
1	o	10	LEU	C-O	-5.58	1.17	1.24
1	B	94	GLU	C-O	-5.58	1.17	1.24
1	j	43	HIS	C-O	-5.58	1.17	1.24
1	V	142	ASP	C-O	-5.57	1.17	1.24
1	L	62	ILE	C-O	-5.57	1.17	1.24
1	L	117	ALA	C-O	-5.57	1.17	1.24
1	i	56	GLU	C-O	-5.57	1.17	1.24
1	U	85	GLU	C-O	-5.57	1.17	1.24
1	V	11	LEU	C-O	-5.57	1.17	1.24
1	O	135	GLU	C-O	-5.57	1.17	1.24
1	C	63	LEU	C-O	-5.57	1.17	1.24
1	K	91	LEU	C-O	-5.57	1.17	1.24
1	S	25	TYR	C-O	-5.57	1.17	1.24
1	D	135	GLU	C-O	-5.56	1.17	1.24
1	n	128	GLU	C-O	-5.56	1.17	1.24
1	r	27	LEU	C-O	-5.56	1.17	1.24
1	F	2	GLN	C-O	-5.56	1.17	1.24
1	M	51	GLU	C-O	-5.56	1.17	1.24
1	G	135	GLU	C-O	-5.56	1.17	1.24
1	K	146	GLU	C-O	-5.56	1.17	1.24
1	S	85	GLU	C-O	-5.56	1.17	1.24
1	h	109	ARG	C-O	-5.56	1.17	1.24
1	G	27	LEU	C-O	-5.56	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	127	GLU	C-O	-5.56	1.17	1.24
1	V	117	ALA	CA-CB	-5.56	1.44	1.53
1	b	26	PHE	C-O	-5.56	1.17	1.24
1	L	26	PHE	C-O	-5.56	1.17	1.24
1	P	58	ILE	C-O	-5.56	1.17	1.24
1	V	29	SER	C-O	-5.56	1.17	1.24
1	X	118	VAL	C-O	-5.55	1.17	1.24
1	t	48	SER	C-O	-5.55	1.17	1.24
1	W	130	HIS	C-O	-5.55	1.17	1.24
1	G	112	GLN	C-O	-5.55	1.16	1.23
1	G	118	VAL	C-O	-5.55	1.17	1.24
1	R	92	ALA	C-O	-5.55	1.17	1.24
1	k	118	VAL	C-O	-5.55	1.17	1.24
1	w	41	ALA	CA-CB	-5.55	1.44	1.53
1	A	79	ILE	CA-CB	-5.55	1.47	1.53
1	C	102	LYS	C-O	-5.55	1.19	1.24
1	G	48	SER	C-O	-5.55	1.17	1.24
1	P	105	ILE	C-O	-5.55	1.17	1.24
1	P	135	GLU	C-O	-5.55	1.17	1.24
1	T	26	PHE	C-O	-5.55	1.17	1.24
1	X	21	ALA	C-O	-5.55	1.17	1.24
1	b	54	HIS	C-O	-5.55	1.17	1.24
1	w	51	GLU	C-O	-5.55	1.17	1.24
1	A	142	ASP	C-O	-5.55	1.17	1.24
1	u	132	ASP	C-O	-5.55	1.17	1.24
1	w	4	ASP	C-O	-5.55	1.16	1.24
1	q	149	TYR	C-O	-5.55	1.17	1.24
1	I	118	VAL	C-O	-5.54	1.17	1.24
1	U	119	LEU	C-O	-5.54	1.17	1.24
1	W	14	GLN	C-O	-5.54	1.17	1.24
1	g	54	HIS	C-O	-5.54	1.17	1.24
1	K	119	LEU	C-O	-5.54	1.17	1.24
1	g	62	ILE	C-O	-5.54	1.17	1.24
1	p	149	TYR	C-O	-5.54	1.17	1.24
1	t	79	ILE	C-O	-5.54	1.18	1.24
1	w	150	SER	C-O	-5.54	1.17	1.24
1	X	137	GLN	C-O	-5.54	1.17	1.24
1	U	91	LEU	C-O	-5.54	1.17	1.24
1	h	130	HIS	C-O	-5.54	1.17	1.24
1	F	92	ALA	CA-CB	-5.54	1.44	1.53
1	O	122	LYS	C-O	-5.54	1.17	1.24
1	t	149	TYR	C-O	-5.54	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	156	ARG	C-O	-5.54	1.19	1.24
1	c	22	ILE	C-O	-5.54	1.17	1.24
1	v	140	LEU	C-O	-5.54	1.17	1.24
1	w	31	MET	C-O	-5.54	1.17	1.24
1	D	84	ARG	C-O	-5.53	1.17	1.24
1	E	151	ALA	C-O	-5.53	1.17	1.24
1	I	104	GLY	C-O	-5.53	1.17	1.23
1	b	126	ASP	C-O	-5.53	1.17	1.24
1	w	141	MET	C-O	-5.53	1.17	1.24
1	X	64	LEU	C-O	-5.53	1.17	1.24
1	m	143	LYS	C-O	-5.53	1.17	1.24
1	Q	134	LEU	C-O	-5.53	1.17	1.24
1	k	138	LEU	C-O	-5.53	1.17	1.24
1	v	115	THR	C-O	-5.53	1.17	1.24
1	A	78	ARG	C-O	-5.53	1.17	1.24
1	C	125	ALA	CA-CB	-5.53	1.44	1.53
1	X	62	ILE	C-O	-5.53	1.17	1.24
1	G	11	LEU	C-O	-5.53	1.17	1.24
1	L	15	LEU	C-O	-5.53	1.17	1.24
1	O	147	GLU	C-O	-5.53	1.17	1.24
1	n	96	ASP	C-O	-5.53	1.17	1.24
1	a	94	GLU	C-O	-5.52	1.17	1.24
1	c	52	MET	C-O	-5.52	1.17	1.24
1	l	2	GLN	C-O	-5.52	1.17	1.24
1	B	4	ASP	C-O	-5.52	1.16	1.24
1	I	117	ALA	C-O	-5.52	1.17	1.24
1	W	125	ALA	C-O	-5.52	1.17	1.24
1	A	154	VAL	C-O	-5.52	1.17	1.23
1	F	56	GLU	C-O	-5.52	1.17	1.24
1	M	25	TYR	C-O	-5.52	1.17	1.24
1	Q	46	ALA	C-O	-5.52	1.17	1.24
1	b	87	PHE	C-O	-5.52	1.17	1.24
1	v	130	HIS	C-O	-5.52	1.17	1.24
1	V	46	ALA	C-O	-5.52	1.17	1.24
1	v	22	ILE	C-O	-5.52	1.17	1.24
1	K	95	TYR	C-O	-5.51	1.17	1.24
1	R	114	THR	N-CA	-5.51	1.39	1.46
1	H	84	ARG	C-O	-5.51	1.17	1.24
1	N	150	SER	C-O	-5.51	1.17	1.24
1	U	102	LYS	CA-C	5.51	1.59	1.52
1	b	99	ASN	C-O	-5.51	1.17	1.24
1	i	24	GLN	C-O	-5.51	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	i	123	ILE	C-O	-5.51	1.17	1.24
1	n	19	LEU	C-O	-5.51	1.17	1.24
1	s	74	ILE	C-O	-5.51	1.18	1.24
1	v	117	ALA	C-O	-5.51	1.17	1.24
1	H	88	GLU	C-O	-5.51	1.17	1.24
1	n	61	ARG	C-O	-5.51	1.17	1.24
1	w	133	TYR	C-O	-5.51	1.17	1.24
1	k	122	LYS	C-O	-5.50	1.17	1.24
1	C	41	ALA	C-O	-5.50	1.17	1.24
1	K	97	VAL	C-O	-5.50	1.18	1.24
1	M	135	GLU	C-O	-5.50	1.17	1.24
1	p	85	GLU	C-O	-5.50	1.17	1.24
1	V	39	GLU	C-O	-5.50	1.17	1.24
1	k	61	ARG	C-O	-5.50	1.17	1.24
1	G	73	ARG	C-O	-5.50	1.17	1.23
1	J	44	THR	C-O	-5.50	1.17	1.24
1	X	94	GLU	C-O	-5.50	1.17	1.24
1	h	127	GLU	C-O	-5.50	1.17	1.24
1	v	55	ALA	C-O	-5.50	1.17	1.24
1	D	29	SER	C-O	-5.50	1.17	1.24
1	S	43	HIS	C-O	-5.50	1.17	1.24
1	f	48	SER	C-O	-5.50	1.17	1.24
1	l	5	PRO	C-O	-5.50	1.17	1.24
1	u	151	ALA	C-O	-5.50	1.17	1.24
1	T	52	MET	C-O	-5.50	1.17	1.24
1	X	127	GLU	C-O	-5.50	1.17	1.24
1	F	23	ASN	C-O	-5.49	1.17	1.24
1	S	76	SER	C-O	-5.49	1.17	1.24
1	b	139	GLU	C-O	-5.49	1.17	1.24
1	A	59	THR	C-O	-5.49	1.17	1.24
1	F	62	ILE	C-O	-5.49	1.17	1.24
1	S	149	TYR	C-O	-5.49	1.17	1.24
1	k	48	SER	C-O	-5.49	1.17	1.24
1	J	62	ILE	C-O	-5.49	1.17	1.24
1	O	126	ASP	C-O	-5.49	1.17	1.24
1	Q	24	GLN	C-O	-5.49	1.17	1.24
1	h	23	ASN	C-O	-5.49	1.17	1.24
1	K	17	SER	C-O	-5.49	1.17	1.24
1	c	59	THR	C-O	-5.49	1.17	1.24
1	l	92	ALA	C-O	-5.49	1.17	1.24
1	n	129	GLU	C-O	-5.49	1.17	1.24
1	F	137	GLN	C-O	-5.49	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	141	MET	C-O	-5.49	1.17	1.24
1	S	139	GLU	C-O	-5.48	1.17	1.24
1	T	47	GLU	C-O	-5.48	1.17	1.24
1	v	83	LEU	C-O	-5.48	1.17	1.24
1	x	22	ILE	CA-CB	-5.48	1.48	1.54
1	x	38	THR	C-O	-5.48	1.17	1.24
1	x	125	ALA	CA-CB	-5.48	1.44	1.53
1	j	85	GLU	C-O	-5.48	1.17	1.24
1	G	12	ASN	C-O	-5.48	1.17	1.24
1	b	106	VAL	C-O	-5.48	1.17	1.24
1	o	96	ASP	C-O	-5.48	1.17	1.24
1	t	41	ALA	CA-CB	-5.48	1.44	1.53
1	B	42	ALA	CA-CB	-5.48	1.44	1.53
1	E	116	SER	C-O	-5.48	1.17	1.24
1	m	154	VAL	C-O	-5.48	1.17	1.24
1	w	142	ASP	C-O	-5.48	1.17	1.24
1	p	45	ARG	C-O	-5.48	1.17	1.24
1	q	15	LEU	C-O	-5.48	1.17	1.24
1	E	41	ALA	CA-CB	-5.47	1.44	1.53
1	O	15	LEU	C-O	-5.47	1.17	1.24
1	X	76	SER	C-O	-5.47	1.17	1.24
1	r	58	ILE	C-O	-5.47	1.17	1.24
1	s	23	ASN	C-O	-5.47	1.17	1.24
1	T	33	ASP	C-O	-5.47	1.17	1.24
1	e	64	LEU	C-O	-5.47	1.17	1.24
1	n	136	THR	C-O	-5.47	1.17	1.24
1	s	68	LEU	C-O	-5.47	1.18	1.24
1	G	126	ASP	C-O	-5.47	1.17	1.24
1	X	88	GLU	C-O	-5.47	1.17	1.24
1	P	149	TYR	C-O	-5.47	1.17	1.24
1	s	11	LEU	C-O	-5.47	1.17	1.24
1	K	103	PRO	C-O	-5.47	1.17	1.24
1	U	52	MET	C-O	-5.47	1.17	1.24
1	V	134	LEU	C-O	-5.47	1.17	1.24
1	X	114	THR	C-O	-5.47	1.17	1.24
1	M	148	LEU	C-O	-5.46	1.17	1.24
1	I	18	GLU	C-O	-5.46	1.17	1.24
1	a	8	LEU	C-O	-5.46	1.17	1.24
1	l	116	SER	C-O	-5.46	1.17	1.24
1	X	33	ASP	C-O	-5.46	1.17	1.24
1	l	146	GLU	C-O	-5.46	1.17	1.24
1	H	106	VAL	C-O	-5.46	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	84	ARG	C-O	-5.46	1.17	1.24
1	T	58	ILE	CG1-CD1	-5.46	1.30	1.51
1	l	58	ILE	C-O	-5.46	1.18	1.24
1	t	50	ASP	C-O	-5.46	1.17	1.24
1	I	115	THR	C-O	-5.46	1.17	1.24
1	f	32	GLN	C-O	-5.46	1.17	1.24
1	g	129	GLU	C-O	-5.46	1.17	1.24
1	n	138	LEU	C-O	-5.46	1.17	1.24
1	v	129	GLU	C-O	-5.46	1.17	1.24
1	I	45	ARG	C-O	-5.45	1.17	1.24
1	h	83	LEU	C-O	-5.45	1.17	1.24
1	Q	89	ALA	C-O	-5.45	1.17	1.24
1	v	32	GLN	C-O	-5.45	1.17	1.24
1	I	130	HIS	C-O	-5.45	1.17	1.24
1	P	34	ASN	C-O	-5.45	1.17	1.24
1	b	16	THR	C-O	-5.45	1.17	1.24
1	O	42	ALA	C-O	-5.45	1.17	1.24
1	l	29	SER	C-O	-5.45	1.17	1.24
1	u	27	LEU	C-O	-5.45	1.17	1.24
1	C	94	GLU	C-O	-5.45	1.17	1.24
1	I	62	ILE	C-O	-5.45	1.18	1.24
1	O	58	ILE	C-O	-5.45	1.17	1.24
1	r	69	PRO	C-O	-5.45	1.17	1.23
1	t	110	GLU	C-O	-5.45	1.17	1.24
1	x	122	LYS	C-O	-5.45	1.17	1.24
1	A	42	ALA	CA-CB	-5.44	1.44	1.53
1	n	47	GLU	C-O	-5.44	1.17	1.24
1	Q	14	GLN	C-O	-5.44	1.17	1.24
1	t	125	ALA	C-O	-5.44	1.17	1.24
1	u	31	MET	C-O	-5.44	1.17	1.24
1	n	63	LEU	C-O	-5.44	1.17	1.24
1	L	130	HIS	C-O	-5.44	1.17	1.24
1	a	97	VAL	C-O	-5.44	1.18	1.24
1	s	2	GLN	C-O	-5.44	1.17	1.24
1	w	60	ASP	C-O	-5.44	1.17	1.24
1	s	114	THR	C-O	-5.44	1.17	1.24
1	t	146	GLU	C-O	-5.44	1.17	1.24
1	U	41	ALA	CA-CB	-5.43	1.44	1.53
1	W	56	GLU	C-O	-5.43	1.17	1.24
1	e	135	GLU	C-O	-5.43	1.17	1.24
1	o	21	ALA	C-O	-5.43	1.17	1.24
1	q	106	VAL	C-O	-5.43	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	134	LEU	C-O	-5.43	1.17	1.24
1	J	32	GLN	C-O	-5.43	1.17	1.24
1	K	23	ASN	C-O	-5.43	1.17	1.24
1	D	103	PRO	C-O	-5.43	1.17	1.24
1	n	10	LEU	C-O	-5.43	1.17	1.24
1	H	125	ALA	C-O	-5.43	1.17	1.24
1	K	151	ALA	C-O	-5.43	1.17	1.24
1	a	119	LEU	C-O	-5.43	1.17	1.24
1	c	32	GLN	C-O	-5.43	1.17	1.24
1	G	65	LEU	C-O	-5.43	1.16	1.24
1	b	61	ARG	C-O	-5.43	1.17	1.24
1	c	30	LYS	C-O	-5.43	1.17	1.24
1	s	59	THR	C-O	-5.43	1.17	1.24
1	p	147	GLU	C-O	-5.42	1.17	1.24
1	q	92	ALA	C-O	-5.42	1.17	1.24
1	A	136	THR	C-O	-5.42	1.17	1.24
1	E	139	GLU	C-O	-5.42	1.17	1.24
1	d	26	PHE	C-O	-5.42	1.17	1.24
1	C	52	MET	C-O	-5.42	1.17	1.24
1	K	137	GLN	C-O	-5.42	1.17	1.24
1	F	69	PRO	C-O	-5.42	1.16	1.23
1	I	102	LYS	C-O	-5.42	1.19	1.24
1	W	50	ASP	C-O	-5.42	1.17	1.24
1	i	150	SER	C-O	-5.42	1.17	1.24
1	s	124	VAL	C-O	-5.42	1.17	1.24
1	x	133	TYR	C-O	-5.42	1.17	1.24
1	D	14	GLN	C-O	-5.42	1.17	1.24
1	D	108	CYS	C-O	-5.42	1.17	1.24
1	i	79	ILE	C-O	-5.42	1.18	1.24
1	N	130	HIS	C-O	-5.42	1.17	1.24
1	G	124	VAL	C-O	-5.42	1.18	1.24
1	K	28	HIS	C-O	-5.42	1.17	1.24
1	N	69	PRO	C-O	-5.41	1.17	1.23
1	x	156	ARG	C-O	-5.41	1.18	1.24
1	V	136	THR	C-O	-5.41	1.17	1.24
1	f	146	GLU	C-O	-5.41	1.17	1.24
1	K	56	GLU	C-O	-5.41	1.17	1.24
1	Q	102	LYS	C-O	-5.41	1.19	1.24
1	t	134	LEU	C-O	-5.41	1.17	1.24
1	B	41	ALA	C-O	-5.40	1.17	1.24
1	E	21	ALA	CA-CB	-5.40	1.44	1.53
1	P	107	MET	C-O	-5.40	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	133	TYR	C-O	-5.40	1.17	1.24
1	X	86	GLN	C-O	-5.40	1.17	1.24
1	b	46	ALA	C-O	-5.40	1.17	1.24
1	g	10	LEU	C-O	-5.40	1.17	1.24
1	p	82	THR	C-O	-5.40	1.17	1.23
1	C	141	MET	C-O	-5.40	1.17	1.24
1	v	27	LEU	C-O	-5.40	1.17	1.24
1	D	41	ALA	C-O	-5.40	1.17	1.24
1	d	15	LEU	C-O	-5.40	1.17	1.24
1	p	114	THR	C-O	-5.40	1.17	1.24
1	t	31	MET	C-O	-5.40	1.17	1.24
1	T	69	PRO	C-O	-5.40	1.17	1.23
1	W	4	ASP	C-O	-5.40	1.17	1.24
1	e	53	ARG	C-O	-5.40	1.17	1.24
1	j	96	ASP	C-O	-5.40	1.17	1.24
1	u	102	LYS	C-O	-5.40	1.19	1.24
1	e	61	ARG	C-O	-5.40	1.17	1.24
1	E	99	ASN	C-O	-5.39	1.17	1.24
1	U	83	LEU	C-O	-5.39	1.17	1.24
1	v	72	GLN	C-O	-5.39	1.17	1.24
1	U	17	SER	C-O	-5.39	1.17	1.24
1	g	135	GLU	C-O	-5.39	1.17	1.24
1	B	30	LYS	C-O	-5.39	1.18	1.24
1	G	47	GLU	C-O	-5.39	1.17	1.24
1	L	82	THR	C-O	-5.39	1.17	1.23
1	M	46	ALA	CA-CB	-5.39	1.44	1.53
1	N	46	ALA	CA-CB	-5.39	1.44	1.53
1	h	88	GLU	C-O	-5.39	1.17	1.24
1	t	54	HIS	C-O	-5.39	1.18	1.24
1	u	26	PHE	C-O	-5.39	1.17	1.24
1	C	17	SER	C-O	-5.39	1.18	1.24
1	E	72	GLN	C-O	-5.39	1.17	1.24
1	T	109	ARG	C-O	-5.39	1.17	1.24
1	U	92	ALA	C-O	-5.39	1.17	1.24
1	J	142	ASP	C-O	-5.39	1.17	1.24
1	L	25	TYR	C-O	-5.39	1.18	1.24
1	k	51	GLU	C-O	-5.39	1.17	1.24
1	v	53	ARG	C-O	-5.39	1.17	1.24
1	B	46	ALA	CA-CB	-5.39	1.44	1.53
1	D	53	ARG	C-O	-5.39	1.17	1.24
1	G	23	ASN	C-O	-5.39	1.18	1.24
1	N	49	PHE	C-O	-5.39	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	41	ALA	CA-CB	-5.39	1.44	1.53
1	X	140	LEU	C-O	-5.39	1.17	1.24
1	h	82	THR	C-O	-5.38	1.17	1.23
1	x	77	LEU	C-O	-5.38	1.17	1.23
1	I	119	LEU	C-O	-5.38	1.17	1.24
1	m	41	ALA	CA-CB	-5.38	1.44	1.53
1	u	10	LEU	C-O	-5.38	1.18	1.24
1	L	79	ILE	C-O	-5.38	1.18	1.24
1	T	126	ASP	C-O	-5.38	1.17	1.24
1	H	117	ALA	C-O	-5.38	1.17	1.24
1	j	118	VAL	C-O	-5.38	1.17	1.24
1	b	121	GLU	C-O	-5.38	1.17	1.24
1	r	90	ASP	C-O	-5.38	1.17	1.24
1	G	22	ILE	C-O	-5.38	1.18	1.24
1	I	123	ILE	C-O	-5.38	1.17	1.24
1	J	109	ARG	C-O	-5.38	1.17	1.24
1	e	99	ASN	C-O	-5.38	1.17	1.24
1	n	114	THR	C-O	-5.38	1.17	1.24
1	X	119	LEU	C-O	-5.38	1.18	1.24
1	K	29	SER	C-O	-5.37	1.17	1.24
1	K	147	GLU	C-O	-5.37	1.17	1.24
1	P	48	SER	C-O	-5.37	1.17	1.24
1	n	122	LYS	C-O	-5.37	1.17	1.24
1	G	117	ALA	CA-CB	-5.37	1.45	1.53
1	R	40	LEU	C-O	-5.37	1.17	1.24
1	V	102	LYS	N-CA	-5.37	1.41	1.46
1	a	44	THR	C-O	-5.37	1.17	1.24
1	v	49	PHE	C-O	-5.37	1.17	1.24
1	x	39	GLU	C-O	-5.37	1.17	1.24
1	q	119	LEU	C-O	-5.37	1.17	1.24
1	R	46	ALA	C-O	-5.37	1.17	1.24
1	n	18	GLU	C-O	-5.37	1.18	1.24
1	s	25	TYR	C-O	-5.37	1.17	1.24
1	s	125	ALA	C-O	-5.37	1.18	1.24
1	x	87	PHE	C-O	-5.37	1.17	1.24
1	C	140	LEU	C-O	-5.37	1.17	1.24
1	X	51	GLU	C-O	-5.37	1.17	1.24
1	o	100	ARG	C-O	-5.37	1.17	1.24
1	B	121	GLU	C-O	-5.37	1.17	1.24
1	F	94	GLU	C-O	-5.37	1.17	1.24
1	i	74	ILE	C-O	-5.37	1.18	1.24
1	o	122	LYS	C-O	-5.37	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	125	ALA	CA-CB	-5.36	1.45	1.53
1	X	113	ASP	C-O	-5.36	1.16	1.23
1	c	8	LEU	N-CA	-5.36	1.39	1.46
1	K	100	ARG	C-O	-5.36	1.17	1.24
1	D	62	ILE	C-O	-5.36	1.17	1.24
1	J	102	LYS	C-O	-5.36	1.19	1.24
1	K	26	PHE	C-O	-5.36	1.17	1.24
1	m	92	ALA	CA-CB	-5.36	1.45	1.53
1	n	89	ALA	C-O	-5.36	1.17	1.24
1	F	12	ASN	C-O	-5.36	1.17	1.24
1	G	5	PRO	C-O	-5.36	1.17	1.24
1	v	134	LEU	C-O	-5.36	1.18	1.24
1	V	139	GLU	C-O	-5.36	1.17	1.24
1	a	17	SER	C-O	-5.36	1.17	1.24
1	f	125	ALA	CA-CB	-5.36	1.45	1.53
1	o	40	LEU	C-O	-5.36	1.17	1.24
1	x	119	LEU	C-O	-5.36	1.18	1.24
1	k	88	GLU	C-O	-5.36	1.17	1.24
1	t	9	ARG	C-O	-5.35	1.17	1.24
1	M	63	LEU	C-O	-5.35	1.18	1.24
1	u	117	ALA	C-O	-5.35	1.17	1.24
1	A	148	LEU	C-O	-5.35	1.17	1.24
1	c	117	ALA	C-O	-5.35	1.18	1.24
1	v	51	GLU	C-O	-5.35	1.17	1.24
1	V	148	LEU	C-O	-5.35	1.17	1.24
1	g	113	ASP	C-O	-5.35	1.15	1.23
1	u	150	SER	C-O	-5.35	1.17	1.24
1	C	47	GLU	C-O	-5.35	1.17	1.24
1	K	25	TYR	C-O	-5.35	1.17	1.24
1	M	2	GLN	C-O	-5.35	1.18	1.24
1	W	91	LEU	C-O	-5.35	1.17	1.24
1	c	88	GLU	C-O	-5.35	1.17	1.24
1	v	56	GLU	C-O	-5.35	1.17	1.24
1	P	21	ALA	C-O	-5.35	1.18	1.24
1	Q	151	ALA	CA-CB	-5.35	1.44	1.53
1	O	121	GLU	C-O	-5.34	1.17	1.24
1	X	126	ASP	C-O	-5.34	1.17	1.24
1	g	7	VAL	C-O	-5.34	1.18	1.24
1	k	80	GLY	C-O	-5.34	1.18	1.23
1	m	22	ILE	C-O	-5.34	1.18	1.24
1	A	132	ASP	C-O	-5.34	1.17	1.24
1	J	88	GLU	C-O	-5.34	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	123	ILE	C-O	-5.34	1.18	1.24
1	N	60	ASP	C-O	-5.34	1.17	1.24
1	U	131	ILE	C-O	-5.34	1.18	1.24
1	x	151	ALA	CA-CB	-5.34	1.44	1.53
1	D	50	ASP	C-O	-5.34	1.17	1.24
1	J	17	SER	C-O	-5.34	1.17	1.24
1	S	121	GLU	C-O	-5.34	1.17	1.24
1	F	46	ALA	CA-CB	-5.34	1.45	1.53
1	I	51	GLU	C-O	-5.34	1.17	1.24
1	p	115	THR	C-O	-5.34	1.18	1.24
1	M	119	LEU	C-O	-5.33	1.17	1.24
1	P	132	ASP	C-O	-5.33	1.18	1.24
1	P	85	GLU	C-O	-5.33	1.17	1.24
1	V	83	LEU	C-O	-5.33	1.17	1.24
1	e	57	GLU	C-O	-5.33	1.17	1.24
1	k	6	ASP	C-O	-5.33	1.17	1.24
1	p	53	ARG	C-O	-5.33	1.18	1.24
1	s	140	LEU	C-O	-5.33	1.17	1.24
1	A	151	ALA	C-O	-5.33	1.17	1.24
1	n	86	GLN	N-CA	-5.33	1.40	1.46
1	F	25	TYR	C-O	-5.33	1.18	1.24
1	v	10	LEU	C-O	-5.33	1.17	1.24
1	f	102	LYS	N-CA	-5.33	1.41	1.46
1	f	151	ALA	C-O	-5.33	1.17	1.24
1	a	68	LEU	C-O	-5.33	1.19	1.24
1	c	140	LEU	C-O	-5.33	1.17	1.24
1	o	90	ASP	C-O	-5.33	1.17	1.24
1	P	82	THR	C-O	-5.32	1.17	1.23
1	T	115	THR	C-O	-5.32	1.17	1.24
1	s	62	ILE	C-O	-5.32	1.18	1.24
1	V	5	PRO	C-O	-5.32	1.17	1.24
1	d	21	ALA	C-O	-5.32	1.17	1.24
1	H	20	THR	C-O	-5.32	1.17	1.24
1	M	42	ALA	C-O	-5.32	1.17	1.24
1	M	76	SER	C-O	-5.32	1.17	1.24
1	O	138	LEU	C-O	-5.32	1.17	1.24
1	P	130	HIS	C-O	-5.32	1.17	1.24
1	Q	137	GLN	C-O	-5.32	1.17	1.24
1	j	28	HIS	C-O	-5.32	1.17	1.24
1	k	63	LEU	C-O	-5.32	1.17	1.24
1	i	102	LYS	C-O	-5.32	1.19	1.24
1	k	22	ILE	CA-CB	-5.32	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	k	108	CYS	C-O	-5.32	1.18	1.24
1	l	105	ILE	C-O	-5.32	1.18	1.24
1	m	55	ALA	C-O	-5.32	1.18	1.24
1	m	99	ASN	C-O	-5.32	1.18	1.24
1	v	50	ASP	C-O	-5.32	1.18	1.24
1	x	45	ARG	C-O	-5.32	1.18	1.24
1	S	129	GLU	C-O	-5.31	1.17	1.24
1	V	16	THR	C-O	-5.31	1.18	1.24
1	i	67	GLY	C-O	-5.31	1.17	1.23
1	B	70	ASN	C-O	-5.31	1.17	1.23
1	H	19	LEU	C-O	-5.31	1.18	1.24
1	X	17	SER	C-O	-5.31	1.18	1.24
1	g	32	GLN	C-O	-5.31	1.18	1.24
1	k	150	SER	C-O	-5.31	1.17	1.24
1	m	87	PHE	C-O	-5.31	1.18	1.24
1	u	36	GLY	C-O	-5.31	1.16	1.24
1	M	22	ILE	C-O	-5.31	1.18	1.24
1	j	127	GLU	C-O	-5.31	1.17	1.24
1	j	149	TYR	C-O	-5.31	1.18	1.24
1	C	89	ALA	CA-CB	-5.31	1.45	1.53
1	F	63	LEU	C-O	-5.31	1.17	1.24
1	H	48	SER	C-O	-5.31	1.18	1.24
1	k	68	LEU	C-O	-5.31	1.18	1.24
1	P	38	THR	C-O	-5.31	1.18	1.24
1	f	79	ILE	C-O	-5.31	1.17	1.24
1	o	22	ILE	C-O	-5.31	1.18	1.24
1	a	23	ASN	C-O	-5.30	1.18	1.24
1	b	92	ALA	CA-CB	-5.30	1.45	1.53
1	p	23	ASN	C-O	-5.30	1.17	1.24
1	q	26	PHE	C-O	-5.30	1.18	1.24
1	A	67	GLY	C-O	-5.30	1.17	1.23
1	N	83	LEU	C-O	-5.30	1.18	1.24
1	U	95	TYR	C-O	-5.30	1.17	1.24
1	g	71	TYR	C-O	-5.30	1.17	1.24
1	A	12	ASN	C-O	-5.30	1.17	1.24
1	U	143	LYS	C-O	-5.30	1.17	1.24
1	o	56	GLU	C-O	-5.30	1.18	1.24
1	x	18	GLU	C-O	-5.30	1.18	1.24
1	L	137	GLN	C-O	-5.30	1.18	1.24
1	L	122	LYS	C-O	-5.30	1.18	1.24
1	b	5	PRO	C-O	-5.30	1.17	1.24
1	m	15	LEU	C-O	-5.30	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	s	138	LEU	C-O	-5.30	1.18	1.24
1	N	124	VAL	C-O	-5.29	1.18	1.24
1	u	56	GLU	C-O	-5.29	1.18	1.24
1	R	88	GLU	C-O	-5.29	1.18	1.24
1	R	140	LEU	C-O	-5.29	1.17	1.24
1	m	122	LYS	C-O	-5.29	1.18	1.24
1	u	77	LEU	C-O	-5.29	1.17	1.23
1	D	6	ASP	C-O	-5.29	1.17	1.24
1	O	25	TYR	C-O	-5.29	1.18	1.24
1	Q	42	ALA	C-O	-5.29	1.18	1.24
1	b	123	ILE	CA-CB	-5.29	1.47	1.54
1	k	128	GLU	C-O	-5.29	1.18	1.24
1	p	102	LYS	C-O	-5.29	1.19	1.24
1	F	50	ASP	C-O	-5.29	1.18	1.24
1	v	39	GLU	C-O	-5.29	1.18	1.24
1	B	115	THR	C-O	-5.29	1.18	1.24
1	H	89	ALA	C-O	-5.29	1.17	1.24
1	M	150	SER	C-O	-5.29	1.17	1.24
1	N	12	ASN	C-O	-5.29	1.17	1.24
1	j	148	LEU	C-O	-5.29	1.18	1.24
1	Q	53	ARG	C-O	-5.29	1.18	1.24
1	w	114	THR	C-O	-5.29	1.18	1.24
1	O	40	LEU	C-O	-5.29	1.18	1.24
1	t	61	ARG	C-O	-5.29	1.17	1.24
1	w	52	MET	C-N	-5.29	1.26	1.33
1	Q	25	TYR	C-O	-5.28	1.18	1.24
1	g	48	SER	C-O	-5.28	1.18	1.24
1	o	51	GLU	C-O	-5.28	1.17	1.24
1	q	118	VAL	C-O	-5.28	1.18	1.24
1	J	90	ASP	C-O	-5.28	1.18	1.24
1	H	114	THR	C-O	-5.28	1.18	1.24
1	P	136	THR	C-O	-5.28	1.17	1.24
1	R	133	TYR	C-O	-5.28	1.18	1.24
1	d	107	MET	C-O	-5.28	1.18	1.24
1	F	11	LEU	C-O	-5.28	1.18	1.24
1	R	130	HIS	C-O	-5.28	1.17	1.24
1	X	120	LEU	C-O	-5.28	1.17	1.24
1	q	117	ALA	C-O	-5.28	1.18	1.24
1	E	127	GLU	C-O	-5.28	1.18	1.24
1	f	137	GLN	C-O	-5.28	1.17	1.24
1	i	92	ALA	CA-CB	-5.28	1.45	1.53
1	l	62	ILE	C-O	-5.28	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	r	62	ILE	C-O	-5.28	1.18	1.24
1	w	117	ALA	CA-CB	-5.28	1.45	1.53
1	x	34	ASN	C-O	-5.28	1.18	1.24
1	R	31	MET	C-O	-5.28	1.17	1.24
1	f	40	LEU	C-O	-5.28	1.18	1.24
1	k	124	VAL	C-O	-5.28	1.18	1.24
1	X	50	ASP	C-O	-5.27	1.18	1.24
1	X	121	GLU	C-O	-5.27	1.18	1.24
1	E	39	GLU	C-O	-5.27	1.18	1.24
1	n	146	GLU	C-O	-5.27	1.18	1.24
1	o	104	GLY	C-O	-5.27	1.17	1.23
1	u	130	HIS	C-O	-5.27	1.18	1.24
1	X	84	ARG	C-O	-5.26	1.18	1.24
1	t	136	THR	C-O	-5.26	1.17	1.24
1	F	31	MET	C-O	-5.26	1.18	1.24
1	M	16	THR	C-O	-5.26	1.18	1.24
1	i	78	ARG	C-O	-5.26	1.17	1.23
1	C	107	MET	C-O	-5.26	1.18	1.24
1	o	119	LEU	C-O	-5.26	1.18	1.24
1	N	117	ALA	C-O	-5.26	1.18	1.24
1	O	44	THR	C-O	-5.26	1.18	1.24
1	U	100	ARG	C-O	-5.26	1.18	1.24
1	k	156	ARG	C-O	-5.26	1.20	1.25
1	n	22	ILE	C-O	-5.26	1.18	1.24
1	B	137	GLN	C-O	-5.25	1.18	1.24
1	b	66	ASP	C-O	-5.25	1.16	1.23
1	F	54	HIS	C-O	-5.25	1.18	1.24
1	I	116	SER	C-O	-5.25	1.18	1.24
1	V	92	ALA	C-O	-5.25	1.18	1.24
1	X	104	GLY	C-O	-5.25	1.17	1.23
1	m	120	LEU	C-O	-5.25	1.17	1.24
1	o	50	ASP	C-O	-5.25	1.18	1.24
1	s	38	THR	C-O	-5.25	1.18	1.24
1	I	52	MET	C-O	-5.25	1.18	1.24
1	O	134	LEU	C-O	-5.25	1.17	1.24
1	X	122	LYS	C-O	-5.25	1.18	1.24
1	c	26	PHE	C-O	-5.25	1.18	1.24
1	t	27	LEU	C-O	-5.25	1.17	1.24
1	d	120	LEU	C-O	-5.25	1.17	1.24
1	C	64	LEU	C-O	-5.25	1.17	1.24
1	E	151	ALA	CA-CB	-5.25	1.44	1.53
1	W	149	TYR	C-O	-5.25	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	r	56	GLU	C-O	-5.25	1.18	1.24
1	u	6	ASP	C-O	-5.25	1.18	1.24
1	H	87	PHE	C-O	-5.25	1.18	1.24
1	m	151	ALA	CA-CB	-5.25	1.44	1.53
1	t	46	ALA	C-O	-5.25	1.18	1.24
1	s	48	SER	C-O	-5.25	1.18	1.24
1	O	123	ILE	C-O	-5.24	1.18	1.24
1	b	19	LEU	C-O	-5.24	1.17	1.24
1	i	64	LEU	C-O	-5.24	1.17	1.24
1	n	23	ASN	C-O	-5.24	1.18	1.24
1	o	69	PRO	C-O	-5.24	1.18	1.23
1	t	115	THR	C-O	-5.24	1.18	1.24
1	v	125	ALA	C-O	-5.24	1.18	1.24
1	w	12	ASN	C-O	-5.24	1.18	1.24
1	x	123	ILE	C-O	-5.24	1.18	1.24
1	N	78	ARG	C-O	-5.24	1.18	1.24
1	Q	5	PRO	C-O	-5.24	1.17	1.24
1	c	9	ARG	C-O	-5.24	1.18	1.24
1	e	62	ILE	C-O	-5.24	1.18	1.24
1	r	146	GLU	C-O	-5.24	1.18	1.24
1	D	12	ASN	C-O	-5.24	1.17	1.24
1	K	132	ASP	C-O	-5.24	1.18	1.24
1	W	59	THR	C-O	-5.24	1.18	1.24
1	l	73	ARG	C-O	-5.24	1.17	1.23
1	l	131	ILE	C-O	-5.24	1.18	1.24
1	t	116	SER	C-O	-5.24	1.18	1.24
1	x	89	ALA	N-CA	-5.24	1.40	1.46
1	S	39	GLU	C-O	-5.24	1.17	1.24
1	T	45	ARG	C-O	-5.24	1.18	1.24
1	M	77	LEU	C-O	-5.24	1.17	1.23
1	e	93	ILE	C-O	-5.24	1.18	1.24
1	f	76	SER	C-O	-5.24	1.17	1.24
1	p	120	LEU	C-O	-5.24	1.18	1.24
1	E	107	MET	C-O	-5.23	1.18	1.24
1	X	10	LEU	C-O	-5.23	1.18	1.24
1	j	19	LEU	C-O	-5.23	1.18	1.24
1	H	99	ASN	C-O	-5.23	1.18	1.24
1	l	124	VAL	C-O	-5.23	1.18	1.24
1	t	16	THR	C-O	-5.23	1.18	1.24
1	L	149	TYR	C-O	-5.23	1.18	1.24
1	N	96	ASP	C-O	-5.23	1.17	1.24
1	O	74	ILE	C-O	-5.23	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	51	GLU	C-O	-5.23	1.18	1.24
1	S	152	GLN	C-O	-5.23	1.17	1.24
1	T	80	GLY	C-O	-5.23	1.16	1.23
1	b	86	GLN	C-O	-5.23	1.17	1.24
1	d	143	LYS	C-O	-5.23	1.18	1.24
1	i	36	GLY	C-O	-5.23	1.16	1.24
1	J	27	LEU	C-O	-5.23	1.18	1.24
1	P	151	ALA	C-O	-5.23	1.17	1.24
1	D	116	SER	C-O	-5.23	1.17	1.24
1	E	78	ARG	C-O	-5.23	1.18	1.24
1	F	95	TYR	C-O	-5.23	1.17	1.24
1	M	7	VAL	C-O	-5.23	1.18	1.24
1	a	134	LEU	C-O	-5.23	1.18	1.24
1	l	99	ASN	C-O	-5.23	1.18	1.24
1	q	43	HIS	C-O	-5.23	1.17	1.24
1	t	62	ILE	C-O	-5.23	1.18	1.24
1	U	42	ALA	C-O	-5.23	1.18	1.24
1	H	34	ASN	C-O	-5.22	1.18	1.24
1	U	24	GLN	C-O	-5.22	1.18	1.24
1	k	149	TYR	C-O	-5.22	1.18	1.24
1	m	92	ALA	C-O	-5.22	1.18	1.24
1	r	117	ALA	C-O	-5.22	1.18	1.24
1	v	98	LEU	C-O	-5.22	1.18	1.24
1	C	125	ALA	C-O	-5.22	1.18	1.24
1	j	64	LEU	C-O	-5.22	1.17	1.24
1	B	33	ASP	C-O	-5.22	1.18	1.24
1	O	12	ASN	C-O	-5.22	1.18	1.24
1	i	111	LYS	C-O	-5.22	1.17	1.24
1	P	17	SER	C-O	-5.22	1.18	1.24
1	b	21	ALA	CA-CB	-5.22	1.44	1.53
1	c	57	GLU	C-O	-5.22	1.18	1.24
1	q	74	ILE	C-O	-5.22	1.18	1.24
1	G	85	GLU	C-O	-5.21	1.18	1.24
1	H	108	CYS	C-O	-5.21	1.18	1.24
1	M	99	ASN	C-O	-5.21	1.18	1.24
1	O	109	ARG	C-O	-5.21	1.18	1.24
1	a	67	GLY	C-O	-5.21	1.17	1.23
1	j	93	ILE	C-O	-5.21	1.18	1.24
1	C	99	ASN	C-O	-5.21	1.18	1.24
1	q	24	GLN	C-O	-5.21	1.18	1.24
1	D	60	ASP	N-CA	-5.21	1.40	1.46
1	E	147	GLU	C-O	-5.21	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	79	ILE	C-O	-5.21	1.18	1.24
1	N	24	GLN	C-O	-5.21	1.18	1.24
1	U	4	ASP	C-O	-5.21	1.17	1.23
1	W	140	LEU	C-O	-5.21	1.18	1.24
1	m	57	GLU	C-O	-5.21	1.18	1.24
1	t	59	THR	C-O	-5.21	1.18	1.24
1	t	106	VAL	C-O	-5.21	1.18	1.24
1	x	115	THR	C-O	-5.21	1.18	1.24
1	A	90	ASP	C-O	-5.21	1.18	1.24
1	N	134	LEU	C-O	-5.21	1.18	1.24
1	i	85	GLU	C-O	-5.21	1.18	1.24
1	j	133	TYR	C-O	-5.21	1.18	1.24
1	u	116	SER	C-O	-5.21	1.18	1.24
1	I	128	GLU	C-O	-5.21	1.18	1.24
1	M	59	THR	C-O	-5.21	1.18	1.24
1	R	89	ALA	C-O	-5.21	1.18	1.24
1	j	45	ARG	C-O	-5.21	1.17	1.24
1	k	103	PRO	C-O	-5.21	1.17	1.24
1	L	29	SER	C-O	-5.21	1.18	1.24
1	N	137	GLN	C-O	-5.21	1.18	1.24
1	r	105	ILE	CA-CB	-5.21	1.48	1.54
1	r	151	ALA	C-O	-5.21	1.17	1.24
1	v	127	GLU	C-O	-5.21	1.18	1.24
1	I	91	LEU	C-O	-5.21	1.18	1.24
1	d	131	ILE	C-O	-5.21	1.18	1.24
1	v	128	GLU	C-O	-5.21	1.18	1.24
1	w	29	SER	C-O	-5.21	1.18	1.24
1	I	21	ALA	C-O	-5.20	1.18	1.24
1	J	91	LEU	C-O	-5.20	1.18	1.24
1	S	126	ASP	C-O	-5.20	1.18	1.24
1	W	30	LYS	C-O	-5.20	1.18	1.24
1	p	22	ILE	C-O	-5.20	1.18	1.24
1	A	60	ASP	C-O	-5.20	1.18	1.24
1	N	59	THR	C-O	-5.20	1.18	1.24
1	b	136	THR	C-O	-5.20	1.18	1.24
1	B	8	LEU	C-O	-5.20	1.18	1.24
1	V	63	LEU	C-O	-5.20	1.17	1.24
1	v	102	LYS	N-CA	-5.20	1.42	1.46
1	H	72	GLN	C-O	-5.20	1.18	1.24
1	Q	17	SER	C-O	-5.20	1.18	1.24
1	d	42	ALA	C-O	-5.20	1.18	1.24
1	d	125	ALA	C-O	-5.20	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	m	81	GLN	C-O	-5.20	1.17	1.24
1	N	20	THR	C-O	-5.20	1.18	1.24
1	R	131	ILE	C-O	-5.20	1.18	1.24
1	i	58	ILE	C-O	-5.20	1.18	1.24
1	i	61	ARG	C-O	-5.20	1.18	1.24
1	l	129	GLU	C-O	-5.20	1.18	1.24
1	N	141	MET	C-O	-5.19	1.18	1.24
1	O	27	LEU	C-O	-5.19	1.18	1.24
1	P	12	ASN	C-O	-5.19	1.18	1.24
1	C	79	ILE	CA-CB	-5.19	1.48	1.54
1	W	114	THR	C-O	-5.19	1.18	1.24
1	p	99	ASN	C-O	-5.19	1.18	1.24
1	t	55	ALA	C-O	-5.19	1.18	1.24
1	C	142	ASP	C-O	-5.19	1.18	1.24
1	U	151	ALA	C-O	-5.19	1.17	1.24
1	g	97	VAL	C-O	-5.19	1.18	1.24
1	I	63	LEU	C-O	-5.19	1.18	1.24
1	U	32	GLN	C-O	-5.19	1.18	1.24
1	d	43	HIS	C-O	-5.19	1.18	1.24
1	r	128	GLU	C-O	-5.19	1.18	1.24
1	G	120	LEU	C-O	-5.19	1.18	1.24
1	H	136	THR	C-O	-5.19	1.18	1.24
1	V	49	PHE	C-O	-5.19	1.18	1.24
1	b	17	SER	C-O	-5.19	1.18	1.24
1	R	119	LEU	C-O	-5.18	1.18	1.24
1	f	119	LEU	C-O	-5.18	1.18	1.24
1	h	79	ILE	C-O	-5.18	1.18	1.24
1	h	89	ALA	C-O	-5.18	1.18	1.24
1	s	65	LEU	C-O	-5.18	1.17	1.24
1	E	102	LYS	C-O	-5.18	1.19	1.24
1	F	141	MET	C-O	-5.18	1.18	1.24
1	N	116	SER	C-O	-5.18	1.18	1.24
1	S	130	HIS	C-O	-5.18	1.18	1.24
1	W	93	ILE	C-O	-5.18	1.18	1.24
1	G	2	GLN	C-O	-5.18	1.18	1.23
1	G	43	HIS	C-O	-5.18	1.18	1.24
1	A	8	LEU	C-O	-5.18	1.18	1.24
1	w	43	HIS	C-O	-5.18	1.18	1.24
1	S	136	THR	C-O	-5.18	1.18	1.24
1	T	151	ALA	C-O	-5.18	1.17	1.24
1	h	92	ALA	C-O	-5.18	1.18	1.24
1	k	29	SER	C-O	-5.18	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	r	21	ALA	C-O	-5.18	1.18	1.24
1	u	14	GLN	C-O	-5.18	1.18	1.24
1	U	141	MET	C-O	-5.17	1.18	1.24
1	m	46	ALA	C-O	-5.17	1.18	1.24
1	M	115	THR	C-O	-5.17	1.18	1.24
1	F	97	VAL	C-O	-5.17	1.18	1.24
1	M	121	GLU	C-O	-5.17	1.18	1.24
1	e	66	ASP	C-O	-5.17	1.16	1.23
1	k	105	ILE	C-O	-5.17	1.18	1.24
1	Q	33	ASP	C-O	-5.17	1.18	1.24
1	m	114	THR	C-O	-5.17	1.18	1.24
1	w	47	GLU	C-O	-5.17	1.18	1.24
1	J	11	LEU	C-O	-5.17	1.18	1.24
1	W	101	LEU	C-O	-5.17	1.17	1.24
1	h	76	SER	C-O	-5.17	1.17	1.24
1	u	129	GLU	C-O	-5.17	1.18	1.24
1	O	110	GLU	C-O	-5.17	1.18	1.24
1	T	116	SER	C-O	-5.17	1.18	1.24
1	h	135	GLU	C-O	-5.17	1.18	1.24
1	H	11	LEU	C-O	-5.17	1.18	1.24
1	e	114	THR	C-O	-5.17	1.18	1.24
1	j	150	SER	C-O	-5.17	1.18	1.24
1	B	7	VAL	CA-CB	5.16	1.60	1.54
1	T	136	THR	C-O	-5.16	1.18	1.24
1	V	47	GLU	C-O	-5.16	1.18	1.24
1	h	117	ALA	C-O	-5.16	1.18	1.24
1	i	117	ALA	C-O	-5.16	1.18	1.24
1	a	107	MET	C-O	-5.16	1.18	1.24
1	k	116	SER	C-O	-5.16	1.18	1.24
1	l	70	ASN	C-O	-5.16	1.17	1.23
1	v	116	SER	C-O	-5.16	1.18	1.24
1	S	24	GLN	C-O	-5.16	1.18	1.24
1	U	148	LEU	C-O	-5.16	1.18	1.24
1	e	143	LYS	C-O	-5.16	1.18	1.24
1	S	100	ARG	C-O	-5.16	1.18	1.24
1	U	45	ARG	C-O	-5.16	1.18	1.24
1	U	128	GLU	C-O	-5.16	1.18	1.24
1	b	33	ASP	C-O	-5.16	1.18	1.24
1	n	148	LEU	C-O	-5.16	1.18	1.24
1	m	125	ALA	CA-CB	-5.15	1.45	1.53
1	G	38	THR	C-O	-5.15	1.18	1.24
1	I	149	TYR	C-O	-5.15	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	151	ALA	CA-CB	-5.15	1.45	1.53
1	j	108	CYS	C-O	-5.15	1.18	1.24
1	p	42	ALA	C-O	-5.15	1.18	1.24
1	S	116	SER	C-O	-5.15	1.18	1.24
1	W	150	SER	C-O	-5.15	1.18	1.24
1	s	121	GLU	C-O	-5.15	1.18	1.24
1	u	79	ILE	C-O	-5.15	1.18	1.24
1	a	40	LEU	C-O	-5.15	1.18	1.24
1	b	13	GLU	C-O	-5.15	1.18	1.24
1	G	84	ARG	C-O	-5.15	1.18	1.24
1	g	85	GLU	C-O	-5.15	1.18	1.24
1	D	92	ALA	C-O	-5.14	1.18	1.24
1	H	63	LEU	C-O	-5.14	1.18	1.24
1	H	137	GLN	C-O	-5.14	1.18	1.24
1	M	55	ALA	C-O	-5.14	1.18	1.24
1	g	119	LEU	C-O	-5.14	1.18	1.24
1	p	156	ARG	CA-C	-5.14	1.46	1.52
1	w	72	GLN	C-O	-5.14	1.18	1.24
1	D	131	ILE	C-O	-5.14	1.18	1.24
1	J	42	ALA	C-O	-5.14	1.18	1.24
1	i	96	ASP	C-O	-5.14	1.18	1.24
1	n	51	GLU	C-O	-5.14	1.18	1.24
1	x	106	VAL	C-O	-5.14	1.18	1.24
1	A	89	ALA	C-O	-5.14	1.18	1.24
1	L	9	ARG	C-O	-5.14	1.18	1.24
1	X	116	SER	C-O	-5.14	1.18	1.24
1	b	57	GLU	C-O	-5.14	1.18	1.24
1	h	20	THR	C-O	-5.14	1.18	1.24
1	n	121	GLU	C-O	-5.14	1.18	1.24
1	w	64	LEU	C-O	-5.14	1.18	1.24
1	J	126	ASP	C-O	-5.14	1.18	1.24
1	O	118	VAL	C-O	-5.14	1.18	1.24
1	Q	85	GLU	C-O	-5.14	1.18	1.24
1	j	65	LEU	C-O	-5.14	1.17	1.24
1	k	27	LEU	C-O	-5.14	1.18	1.24
1	A	15	LEU	C-O	-5.13	1.18	1.24
1	B	102	LYS	N-CA	-5.13	1.41	1.46
1	G	31	MET	C-O	-5.13	1.18	1.24
1	H	128	GLU	C-O	-5.13	1.18	1.24
1	U	68	LEU	C-O	-5.13	1.17	1.24
1	f	36	GLY	C-O	-5.13	1.17	1.24
1	r	83	LEU	C-O	-5.13	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	51	GLU	C-O	-5.13	1.17	1.24
1	a	46	ALA	C-O	-5.13	1.18	1.24
1	j	103	PRO	C-O	-5.13	1.18	1.24
1	l	96	ASP	C-O	-5.13	1.18	1.24
1	w	77	LEU	C-O	-5.13	1.17	1.24
1	I	126	ASP	C-O	-5.13	1.18	1.24
1	m	34	ASN	C-O	-5.13	1.18	1.24
1	F	129	GLU	C-O	-5.13	1.18	1.24
1	M	149	TYR	C-O	-5.13	1.18	1.24
1	f	49	PHE	C-O	-5.13	1.17	1.24
1	i	93	ILE	C-O	-5.13	1.17	1.24
1	B	84	ARG	C-O	-5.13	1.18	1.24
1	F	43	HIS	C-O	-5.13	1.18	1.24
1	e	11	LEU	C-O	-5.13	1.18	1.24
1	e	41	ALA	C-O	-5.13	1.18	1.24
1	v	112	GLN	C-O	-5.13	1.16	1.23
1	W	8	LEU	C-O	-5.12	1.18	1.24
1	F	33	ASP	C-O	-5.12	1.18	1.24
1	M	100	ARG	C-O	-5.12	1.18	1.24
1	P	99	ASN	C-O	-5.12	1.18	1.24
1	b	31	MET	C-O	-5.12	1.18	1.24
1	p	72	GLN	C-O	-5.12	1.17	1.24
1	C	122	LYS	C-O	-5.12	1.18	1.24
1	d	148	LEU	C-O	-5.12	1.18	1.24
1	f	58	ILE	C-O	-5.12	1.18	1.24
1	M	87	PHE	C-O	-5.12	1.18	1.24
1	t	7	VAL	C-O	-5.12	1.18	1.24
1	I	41	ALA	C-O	-5.12	1.18	1.24
1	N	140	LEU	C-O	-5.12	1.18	1.24
1	p	132	ASP	C-O	-5.12	1.18	1.24
1	e	5	PRO	C-O	-5.12	1.18	1.24
1	h	12	ASN	C-O	-5.12	1.18	1.24
1	A	111	LYS	C-O	-5.12	1.17	1.24
1	G	140	LEU	C-O	-5.12	1.18	1.24
1	i	127	GLU	C-O	-5.12	1.18	1.24
1	k	77	LEU	C-O	-5.12	1.17	1.23
1	m	58	ILE	CG1-CD1	-5.12	1.31	1.51
1	o	16	THR	C-O	-5.12	1.18	1.24
1	p	59	THR	C-O	-5.12	1.18	1.24
1	E	77	LEU	C-O	-5.11	1.17	1.23
1	T	22	ILE	C-O	-5.11	1.18	1.24
1	W	117	ALA	C-O	-5.11	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	j	13	GLU	C-O	-5.11	1.18	1.24
1	t	64	LEU	C-O	-5.11	1.18	1.24
1	I	97	VAL	C-O	-5.11	1.18	1.24
1	L	83	LEU	C-O	-5.11	1.18	1.24
1	Q	21	ALA	C-O	-5.11	1.17	1.24
1	l	119	LEU	C-O	-5.11	1.18	1.24
1	p	34	ASN	C-O	-5.11	1.17	1.24
1	p	76	SER	C-O	-5.11	1.17	1.24
1	H	43	HIS	C-O	-5.11	1.18	1.24
1	Q	132	ASP	C-O	-5.11	1.18	1.24
1	V	150	SER	C-O	-5.11	1.17	1.24
1	l	8	LEU	C-O	-5.11	1.18	1.24
1	c	50	ASP	C-O	-5.11	1.18	1.24
1	V	61	ARG	C-O	-5.11	1.18	1.24
1	l	15	LEU	C-O	-5.11	1.18	1.24
1	n	156	ARG	C-O	-5.11	1.20	1.25
1	o	46	ALA	C-O	-5.10	1.18	1.24
1	P	40	LEU	C-O	-5.10	1.18	1.24
1	T	131	ILE	C-O	-5.10	1.18	1.24
1	x	21	ALA	C-O	-5.10	1.18	1.24
1	V	41	ALA	CA-CB	-5.10	1.45	1.53
1	n	106	VAL	CA-CB	-5.10	1.48	1.54
1	F	61	ARG	C-O	-5.10	1.18	1.24
1	H	131	ILE	C-O	-5.10	1.18	1.24
1	m	47	GLU	C-O	-5.10	1.18	1.24
1	n	130	HIS	C-O	-5.10	1.18	1.24
1	o	85	GLU	C-O	-5.10	1.18	1.24
1	F	66	ASP	C-O	-5.10	1.17	1.23
1	H	9	ARG	C-O	-5.10	1.18	1.24
1	K	51	GLU	C-O	-5.10	1.18	1.24
1	a	87	PHE	C-O	-5.10	1.18	1.24
1	e	27	LEU	C-O	-5.10	1.18	1.24
1	H	66	ASP	C-O	-5.10	1.15	1.24
1	b	129	GLU	C-O	-5.10	1.18	1.24
1	o	144	LEU	C-O	-5.10	1.17	1.24
1	V	141	MET	C-O	-5.09	1.18	1.24
1	q	140	LEU	C-O	-5.09	1.17	1.24
1	t	146	GLU	N-CA	-5.09	1.40	1.46
1	x	49	PHE	C-O	-5.09	1.18	1.24
1	K	94	GLU	C-O	-5.09	1.18	1.24
1	l	72	GLN	C-O	-5.09	1.18	1.24
1	o	6	ASP	C-O	-5.09	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	r	42	ALA	C-O	-5.09	1.17	1.24
1	R	22	ILE	C-O	-5.09	1.18	1.24
1	S	68	LEU	C-O	-5.09	1.18	1.24
1	G	142	ASP	C-O	-5.09	1.18	1.24
1	a	110	GLU	C-O	-5.09	1.17	1.24
1	c	149	TYR	C-O	-5.09	1.18	1.24
1	T	56	GLU	C-O	-5.09	1.18	1.24
1	l	75	GLY	C-O	-5.09	1.17	1.23
1	v	137	GLN	C-O	-5.09	1.18	1.24
1	B	118	VAL	C-O	-5.09	1.18	1.24
1	O	140	LEU	C-O	-5.09	1.17	1.24
1	T	153	CYS	C-O	-5.09	1.17	1.24
1	X	139	GLU	C-O	-5.09	1.18	1.24
1	g	147	GLU	C-O	-5.09	1.18	1.24
1	L	41	ALA	CA-CB	-5.08	1.45	1.53
1	V	98	LEU	C-O	-5.08	1.18	1.24
1	G	95	TYR	C-O	-5.08	1.17	1.24
1	H	55	ALA	C-O	-5.08	1.18	1.24
1	a	146	GLU	C-O	-5.08	1.18	1.24
1	w	151	ALA	CA-CB	-5.08	1.45	1.53
1	n	140	LEU	C-O	-5.08	1.18	1.24
1	A	108	CYS	C-O	-5.08	1.18	1.24
1	K	41	ALA	CA-CB	-5.08	1.45	1.53
1	Q	139	GLU	C-O	-5.08	1.18	1.24
1	e	107	MET	C-O	-5.08	1.18	1.24
1	m	25	TYR	C-O	-5.08	1.18	1.24
1	n	24	GLN	C-O	-5.08	1.18	1.24
1	o	52	MET	C-O	-5.08	1.18	1.24
1	G	102	LYS	C-O	-5.08	1.20	1.24
1	T	130	HIS	C-O	-5.08	1.18	1.24
1	d	158	PRO	C-O	-5.08	1.17	1.23
1	D	9	ARG	C-O	-5.08	1.18	1.24
1	L	22	ILE	C-O	-5.08	1.18	1.24
1	g	64	LEU	C-O	-5.08	1.18	1.24
1	i	129	GLU	C-O	-5.08	1.18	1.24
1	E	97	VAL	C-O	-5.07	1.18	1.24
1	P	84	ARG	C-O	-5.07	1.18	1.24
1	Q	47	GLU	C-O	-5.07	1.17	1.24
1	g	31	MET	C-O	-5.07	1.18	1.24
1	j	95	TYR	C-O	-5.07	1.17	1.24
1	k	39	GLU	C-O	-5.07	1.18	1.24
1	n	9	ARG	C-O	-5.07	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	g	139	GLU	C-O	-5.07	1.18	1.24
1	o	12	ASN	C-O	-5.07	1.18	1.24
1	T	19	LEU	C-O	-5.07	1.18	1.24
1	l	46	ALA	C-O	-5.07	1.18	1.24
1	m	67	GLY	C-O	-5.07	1.16	1.23
1	o	11	LEU	C-O	-5.07	1.18	1.24
1	P	108	CYS	CB-SG	-5.07	1.64	1.81
1	p	106	VAL	C-O	-5.07	1.18	1.24
1	x	41	ALA	C-O	-5.07	1.18	1.24
1	S	77	LEU	C-O	-5.07	1.17	1.23
1	T	105	ILE	C-O	-5.07	1.18	1.24
1	X	110	GLU	C-O	-5.07	1.18	1.24
1	F	58	ILE	C-O	-5.07	1.18	1.24
1	O	34	ASN	C-O	-5.07	1.17	1.24
1	X	87	PHE	C-O	-5.07	1.18	1.24
1	d	50	ASP	C-O	-5.07	1.18	1.24
1	h	99	ASN	C-O	-5.07	1.18	1.24
1	k	21	ALA	CA-CB	-5.07	1.45	1.53
1	x	46	ALA	CA-CB	-5.07	1.45	1.53
1	S	62	ILE	C-O	-5.06	1.18	1.24
1	d	59	THR	C-O	-5.06	1.18	1.24
1	h	114	THR	C-O	-5.06	1.17	1.24
1	R	151	ALA	C-O	-5.06	1.17	1.24
1	b	98	LEU	C-O	-5.06	1.18	1.24
1	i	146	GLU	C-O	-5.06	1.18	1.24
1	j	6	ASP	C-O	-5.06	1.18	1.24
1	u	81	GLN	C-O	-5.06	1.17	1.23
1	E	158	PRO	C-O	-5.06	1.17	1.23
1	F	102	LYS	C-O	-5.06	1.19	1.24
1	L	11	LEU	C-O	-5.06	1.18	1.24
1	b	117	ALA	CA-CB	-5.06	1.45	1.53
1	g	99	ASN	C-O	-5.06	1.18	1.24
1	j	8	LEU	C-O	-5.06	1.18	1.24
1	C	33	ASP	C-O	-5.06	1.18	1.24
1	M	26	PHE	C-O	-5.06	1.18	1.24
1	P	98	LEU	C-O	-5.06	1.18	1.24
1	R	102	LYS	N-CA	-5.06	1.42	1.46
1	d	119	LEU	C-O	-5.06	1.18	1.24
1	n	52	MET	C-O	-5.06	1.18	1.24
1	D	22	ILE	C-O	-5.06	1.18	1.24
1	V	50	ASP	C-O	-5.06	1.18	1.24
1	n	67	GLY	C-O	-5.06	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	g	120	LEU	C-O	-5.05	1.18	1.24
1	u	12	ASN	C-O	-5.05	1.18	1.24
1	U	35	TRP	C-O	-5.05	1.17	1.24
1	F	60	ASP	C-O	-5.05	1.18	1.24
1	i	104	GLY	C-O	-5.05	1.17	1.23
1	v	92	ALA	C-O	-5.05	1.18	1.24
1	G	147	GLU	C-O	-5.05	1.18	1.24
1	T	36	GLY	C-O	-5.05	1.17	1.24
1	a	41	ALA	C-O	-5.05	1.18	1.24
1	a	83	LEU	C-O	-5.05	1.18	1.24
1	g	68	LEU	C-O	-5.05	1.18	1.24
1	o	141	MET	SD-CE	-5.05	1.67	1.79
1	P	30	LYS	C-O	-5.05	1.18	1.24
1	S	137	GLN	C-O	-5.05	1.18	1.24
1	m	38	THR	C-O	-5.05	1.18	1.24
1	n	12	ASN	C-O	-5.05	1.17	1.24
1	W	3	GLY	C-O	-5.04	1.16	1.23
1	k	92	ALA	C-O	-5.04	1.18	1.24
1	q	69	PRO	C-O	-5.04	1.18	1.23
1	u	93	ILE	C-O	-5.04	1.18	1.24
1	v	105	ILE	C-O	-5.04	1.18	1.24
1	G	136	THR	C-O	-5.04	1.18	1.24
1	S	109	ARG	C-O	-5.04	1.18	1.24
1	Q	156	ARG	CA-C	-5.04	1.46	1.52
1	U	28	HIS	C-O	-5.04	1.18	1.24
1	l	60	ASP	C-O	-5.04	1.18	1.24
1	m	19	LEU	C-O	-5.04	1.18	1.24
1	s	86	GLN	C-O	-5.04	1.18	1.24
1	R	51	GLU	C-O	-5.04	1.17	1.24
1	k	100	ARG	C-O	-5.04	1.18	1.24
1	o	5	PRO	C-O	-5.04	1.18	1.24
1	q	23	ASN	C-O	-5.04	1.18	1.24
1	C	32	GLN	C-O	-5.04	1.18	1.24
1	G	6	ASP	C-O	-5.04	1.18	1.24
1	L	158	PRO	C-O	-5.04	1.17	1.23
1	f	85	GLU	C-O	-5.04	1.18	1.24
1	i	12	ASN	C-O	-5.04	1.18	1.24
1	j	116	SER	C-O	-5.04	1.18	1.24
1	k	136	THR	C-O	-5.04	1.18	1.24
1	s	41	ALA	CA-CB	-5.04	1.45	1.53
1	K	41	ALA	C-O	-5.04	1.18	1.24
1	h	42	ALA	C-O	-5.04	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	j	42	ALA	CA-CB	-5.04	1.45	1.53
1	t	105	ILE	C-O	-5.04	1.18	1.24
1	X	57	GLU	C-O	-5.04	1.18	1.24
1	h	106	VAL	C-O	-5.04	1.18	1.24
1	i	68	LEU	C-O	-5.04	1.20	1.25
1	k	72	GLN	C-O	-5.04	1.17	1.24
1	n	95	TYR	C-O	-5.04	1.17	1.24
1	x	146	GLU	C-O	-5.04	1.18	1.24
1	e	12	ASN	C-O	-5.03	1.18	1.24
1	L	68	LEU	C-O	-5.03	1.18	1.24
1	s	62	ILE	N-CA	-5.03	1.40	1.46
1	s	103	PRO	C-O	-5.03	1.18	1.24
1	L	70	ASN	C-O	-5.03	1.18	1.24
1	x	94	GLU	C-O	-5.03	1.18	1.24
1	D	61	ARG	C-O	-5.03	1.18	1.24
1	I	64	LEU	C-O	-5.03	1.17	1.24
1	x	126	ASP	C-O	-5.03	1.18	1.24
1	U	74	ILE	C-O	-5.03	1.19	1.24
1	c	134	LEU	C-O	-5.03	1.18	1.24
1	q	116	SER	C-O	-5.03	1.18	1.24
1	h	10	LEU	C-O	-5.02	1.18	1.24
1	B	79	ILE	C-O	-5.02	1.18	1.24
1	E	9	ARG	C-O	-5.02	1.18	1.24
1	I	114	THR	C-O	-5.02	1.18	1.24
1	a	99	ASN	C-O	-5.02	1.18	1.24
1	p	21	ALA	CA-CB	-5.02	1.45	1.53
1	R	15	LEU	C-O	-5.02	1.18	1.24
1	v	13	GLU	C-O	-5.02	1.18	1.24
1	C	42	ALA	CA-CB	-5.02	1.45	1.53
1	J	120	LEU	C-O	-5.02	1.18	1.24
1	T	16	THR	C-O	-5.02	1.18	1.24
1	j	101	LEU	C-O	-5.02	1.17	1.24
1	B	18	GLU	C-O	-5.02	1.18	1.24
1	Q	95	TYR	C-O	-5.02	1.18	1.24
1	j	56	GLU	C-O	-5.02	1.18	1.24
1	l	77	LEU	C-O	-5.02	1.17	1.23
1	o	45	ARG	C-O	-5.02	1.18	1.24
1	s	60	ASP	C-O	-5.02	1.18	1.24
1	x	117	ALA	C-O	-5.02	1.18	1.24
1	D	119	LEU	C-O	-5.01	1.18	1.24
1	N	120	LEU	C-O	-5.01	1.18	1.24
1	O	39	GLU	C-O	-5.01	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	77	LEU	C-O	-5.01	1.17	1.23
1	k	142	ASP	C-O	-5.01	1.18	1.24
1	E	118	VAL	C-O	-5.01	1.18	1.24
1	x	151	ALA	C-O	-5.01	1.17	1.24
1	A	80	GLY	C-O	-5.01	1.19	1.24
1	N	8	LEU	C-O	-5.01	1.18	1.24
1	P	144	LEU	C-O	-5.01	1.18	1.24
1	h	116	SER	C-O	-5.01	1.18	1.24
1	j	59	THR	C-O	-5.01	1.18	1.24
1	A	69	PRO	C-O	-5.01	1.18	1.23
1	O	130	HIS	C-O	-5.01	1.18	1.24
1	u	24	GLN	C-O	-5.01	1.18	1.24
1	H	89	ALA	CA-CB	-5.01	1.45	1.53
1	P	90	ASP	C-O	-5.01	1.18	1.24
1	Q	122	LYS	C-O	-5.01	1.18	1.24
1	j	92	ALA	C-O	-5.01	1.18	1.24
1	D	150	SER	C-O	-5.01	1.18	1.24
1	L	48	SER	C-O	-5.01	1.18	1.24
1	M	56	GLU	C-O	-5.01	1.18	1.24
1	P	9	ARG	C-O	-5.01	1.18	1.24
1	t	47	GLU	C-O	-5.01	1.18	1.24
1	A	56	GLU	C-O	-5.00	1.18	1.24
1	f	55	ALA	C-O	-5.00	1.18	1.24
1	A	149	TYR	C-O	-5.00	1.18	1.24
1	D	129	GLU	C-O	-5.00	1.18	1.24
1	e	134	LEU	C-O	-5.00	1.18	1.24
1	m	63	LEU	C-O	-5.00	1.18	1.24
1	w	11	LEU	C-O	-5.00	1.18	1.24
1	D	115	THR	C-O	-5.00	1.18	1.24
1	J	150	SER	C-O	-5.00	1.18	1.24
1	T	131	ILE	CG1-CD1	-5.00	1.32	1.51
1	h	8	LEU	C-O	-5.00	1.18	1.24
1	s	105	ILE	C-O	-5.00	1.18	1.24
1	u	21	ALA	C-O	-5.00	1.18	1.24

All (361) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	i	93	ILE	CA-C-N	12.32	141.62	120.68
1	i	93	ILE	C-N-CA	12.32	141.62	120.68
1	N	93	ILE	CA-C-N	-12.29	104.42	120.65
1	N	93	ILE	C-N-CA	-12.29	104.42	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	w	94	GLU	O-C-N	-11.81	109.91	122.07
1	f	127	GLU	O-C-N	11.46	135.21	122.15
1	i	93	ILE	O-C-N	-10.51	109.92	121.80
1	q	94	GLU	O-C-N	-10.33	109.70	122.20
1	h	72	GLN	N-CA-C	10.04	122.30	111.36
1	r	72	GLN	N-CA-C	9.77	122.01	111.36
1	E	127	GLU	O-C-N	9.60	132.08	122.09
1	D	72	GLN	N-CA-C	9.43	121.32	111.14
1	E	72	GLN	N-CA-C	9.10	121.28	111.36
1	E	144	LEU	N-CA-C	8.96	121.12	111.36
1	J	18	GLU	O-C-N	8.95	133.87	122.23
1	S	94	GLU	O-C-N	-8.73	113.01	122.09
1	d	101	LEU	N-CA-C	8.63	121.84	111.82
1	g	101	LEU	N-CA-C	8.43	120.55	111.36
1	R	72	GLN	N-CA-C	8.37	120.48	111.36
1	t	101	LEU	N-CA-C	8.36	120.47	111.36
1	G	101	LEU	N-CA-C	8.35	120.46	111.36
1	B	72	GLN	N-CA-C	8.31	120.42	111.36
1	x	101	LEU	N-CA-C	8.25	121.39	111.82
1	w	72	GLN	N-CA-C	8.19	120.28	111.36
1	F	101	LEU	N-CA-C	8.12	120.21	111.36
1	E	101	LEU	N-CA-C	8.07	120.15	111.36
1	f	126	ASP	CA-C-N	8.06	131.73	120.29
1	f	126	ASP	C-N-CA	8.06	131.73	120.29
1	p	101	LEU	N-CA-C	8.06	121.17	111.82
1	m	100	ARG	N-CA-C	7.99	119.77	111.14
1	P	144	LEU	N-CA-C	7.99	120.06	111.36
1	C	72	GLN	N-CA-C	7.90	119.97	111.36
1	q	142	ASP	N-CA-C	7.89	119.66	111.14
1	R	101	LEU	N-CA-C	7.80	119.86	111.36
1	D	60	ASP	N-CA-C	-7.78	102.75	111.07
1	l	100	ARG	N-CA-C	7.76	119.52	111.14
1	D	145	GLY	N-CA-C	-7.71	103.15	112.48
1	d	72	GLN	N-CA-C	7.63	119.68	111.36
1	c	97	VAL	CB-CA-C	-7.63	102.21	111.97
1	E	34	ASN	N-CA-C	7.62	119.58	111.28
1	G	72	GLN	N-CA-C	7.60	119.65	111.36
1	f	101	LEU	N-CA-C	7.53	119.56	111.36
1	p	51	GLU	O-C-N	7.51	132.40	122.33
1	S	72	GLN	N-CA-C	7.50	119.53	111.36
1	m	144	LEU	N-CA-C	7.50	119.53	111.36
1	b	101	LEU	N-CA-C	7.48	119.51	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	101	LEU	N-CA-C	7.44	120.45	111.82
1	C	144	LEU	N-CA-C	7.42	120.43	111.82
1	v	145	GLY	N-CA-C	-7.38	102.06	111.72
1	F	144	LEU	N-CA-C	7.36	119.38	111.36
1	P	101	LEU	N-CA-C	7.36	119.30	111.28
1	x	145	GLY	N-CA-C	-7.34	102.34	112.18
1	N	72	GLN	N-CA-C	7.34	120.33	111.82
1	J	72	GLN	N-CA-C	7.34	119.36	111.36
1	q	52	MET	N-CA-C	-7.28	103.34	111.28
1	N	143	LYS	N-CA-C	7.21	119.14	111.28
1	F	146	GLU	N-CA-C	7.20	119.13	111.28
1	m	72	GLN	N-CA-C	7.16	119.16	111.36
1	A	156	ARG	CB-CA-C	-7.16	104.00	110.44
1	N	156	ARG	CB-CA-C	-7.16	104.00	110.44
1	H	72	GLN	N-CA-C	7.15	119.16	111.36
1	J	144	LEU	N-CA-C	7.15	121.24	112.23
1	E	142	ASP	N-CA-C	7.15	118.86	111.14
1	X	101	LEU	N-CA-C	7.14	120.10	111.82
1	W	134	LEU	N-CA-C	7.09	118.66	111.07
1	j	145	GLY	N-CA-C	-7.07	103.93	112.48
1	p	146	GLU	N-CA-C	7.05	118.97	111.28
1	d	149	TYR	CA-C-N	7.04	130.28	120.29
1	d	149	TYR	C-N-CA	7.04	130.28	120.29
1	P	142	ASP	N-CA-C	6.97	118.67	111.14
1	H	101	LEU	N-CA-C	6.96	119.89	111.82
1	O	93	ILE	CB-CA-C	6.95	121.82	112.22
1	r	3	GLY	N-CA-C	6.92	121.39	112.54
1	J	101	LEU	N-CA-C	6.88	119.80	111.82
1	a	51	GLU	CB-CG-CD	6.84	124.23	112.60
1	x	125	ALA	CA-C-N	6.83	129.73	120.44
1	x	125	ALA	C-N-CA	6.83	129.73	120.44
1	C	23	ASN	N-CA-C	6.81	118.78	111.36
1	M	2	GLN	N-CA-C	6.80	119.49	108.34
1	S	38	THR	N-CA-C	6.76	118.65	111.28
1	Q	146	GLU	N-CA-C	6.74	118.41	111.14
1	O	72	GLN	N-CA-C	6.72	118.40	111.14
1	Q	101	LEU	N-CA-C	6.67	118.63	111.36
1	M	126	ASP	O-C-N	6.61	129.13	122.12
1	j	100	ARG	N-CA-C	6.61	118.28	111.14
1	W	72	GLN	N-CA-C	6.61	121.55	112.90
1	K	72	GLN	N-CA-C	6.59	118.26	111.14
1	h	96	ASP	N-CA-C	-6.59	104.02	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	72	GLN	N-CA-C	6.58	118.25	111.14
1	t	143	LYS	N-CA-C	6.58	118.54	111.36
1	D	107	MET	N-CA-C	6.54	118.07	111.07
1	b	144	LEU	N-CA-C	6.51	120.97	112.89
1	q	101	LEU	N-CA-C	6.51	119.20	111.71
1	n	146	GLU	N-CA-C	6.51	118.17	111.14
1	W	2	GLN	N-CA-C	6.50	119.75	108.76
1	E	51	GLU	CG-CD-OE2	6.48	133.30	118.40
1	Q	144	LEU	N-CA-C	6.47	118.42	111.36
1	M	100	ARG	N-CA-C	6.47	118.13	111.14
1	M	22	ILE	CB-CA-C	-6.47	103.69	111.97
1	D	101	LEU	N-CA-C	6.46	118.40	111.36
1	S	101	LEU	N-CA-C	6.46	118.40	111.36
1	c	33	ASP	CA-C-N	6.46	128.93	120.28
1	c	33	ASP	C-N-CA	6.46	128.93	120.28
1	f	134	LEU	N-CA-C	6.45	118.31	111.28
1	L	3	GLY	N-CA-C	6.44	121.39	112.37
1	C	142	ASP	N-CA-C	6.42	118.07	111.14
1	T	145	GLY	N-CA-C	-6.40	103.61	112.18
1	F	106	VAL	N-CA-C	-6.37	104.12	110.62
1	R	23	ASN	N-CA-C	6.37	117.89	111.07
1	A	101	LEU	N-CA-C	6.35	119.18	111.82
1	n	101	LEU	N-CA-C	6.33	118.98	111.71
1	j	72	GLN	N-CA-C	6.28	118.20	111.36
1	x	142	ASP	N-CA-C	6.25	117.90	111.14
1	v	153	CYS	N-CA-C	6.23	120.89	113.16
1	c	72	GLN	N-CA-C	6.22	118.14	111.36
1	s	134	LEU	N-CA-C	6.21	117.72	111.07
1	I	101	LEU	N-CA-C	6.21	119.02	111.82
1	w	101	LEU	N-CA-C	6.20	118.12	111.36
1	H	143	LYS	N-CA-C	6.20	118.12	111.36
1	L	144	LEU	N-CA-C	6.18	120.90	113.23
1	a	51	GLU	CG-CD-OE2	6.18	132.62	118.40
1	i	38	THR	N-CA-C	6.16	118.07	111.36
1	A	134	LEU	N-CA-C	6.15	118.06	111.36
1	T	93	ILE	N-CA-C	6.14	116.92	110.72
1	e	101	LEU	N-CA-C	6.14	118.77	111.71
1	g	110	GLU	N-CA-C	-6.13	104.59	111.28
1	u	144	LEU	N-CA-C	6.13	118.93	111.82
1	H	38	THR	N-CA-C	6.12	117.95	111.28
1	c	114	THR	N-CA-C	6.11	117.94	111.28
1	v	101	LEU	N-CA-C	6.09	118.89	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	46	ALA	CA-C-N	6.08	128.43	120.28
1	U	46	ALA	C-N-CA	6.08	128.43	120.28
1	t	25	TYR	O-C-N	-6.06	115.69	122.12
1	M	112	GLN	N-CA-C	6.06	120.04	111.92
1	s	101	LEU	N-CA-C	6.06	118.85	111.82
1	L	4	ASP	CA-C-N	6.04	125.76	119.05
1	L	4	ASP	C-N-CA	6.04	125.76	119.05
1	U	146	GLU	N-CA-C	6.04	117.94	111.36
1	M	110	GLU	N-CA-C	6.04	117.94	111.36
1	O	143	LYS	N-CA-C	6.03	117.52	111.07
1	E	126	ASP	CA-C-N	6.02	128.67	120.54
1	E	126	ASP	C-N-CA	6.02	128.67	120.54
1	n	145	GLY	N-CA-C	-6.02	104.12	112.18
1	S	23	ASN	N-CA-C	6.01	117.50	111.07
1	M	120	LEU	N-CA-C	6.00	117.90	111.36
1	j	51	GLU	CG-CD-OE1	5.99	132.19	118.40
1	u	146	GLU	N-CA-C	5.99	117.81	111.28
1	A	100	ARG	N-CA-C	5.99	117.61	111.14
1	T	144	LEU	N-CA-C	5.99	117.89	111.36
1	C	101	LEU	N-CA-C	5.98	117.88	111.36
1	L	145	GLY	N-CA-C	-5.97	104.18	112.18
1	A	146	GLU	N-CA-C	5.96	117.45	111.07
1	j	146	GLU	N-CA-C	5.95	117.44	111.07
1	B	101	LEU	N-CA-C	5.95	117.84	111.36
1	u	100	ARG	N-CA-C	5.94	117.56	111.14
1	W	23	ASN	N-CA-C	5.93	117.42	111.07
1	d	137	GLN	O-C-N	5.92	129.92	122.23
1	n	23	ASN	N-CA-C	5.91	117.40	111.07
1	v	144	LEU	N-CA-C	5.91	117.80	111.36
1	D	2	GLN	N-CA-C	5.91	118.03	108.34
1	U	88	GLU	N-CA-C	5.90	117.79	111.36
1	V	51	GLU	CB-CG-CD	5.90	122.63	112.60
1	a	72	GLN	N-CA-C	5.90	117.79	111.36
1	u	112	GLN	N-CA-C	5.89	119.69	111.74
1	o	146	GLU	N-CA-C	5.88	117.77	111.36
1	M	127	GLU	CA-C-N	5.87	128.43	120.44
1	M	127	GLU	C-N-CA	5.87	128.43	120.44
1	V	72	GLN	N-CA-C	5.87	117.76	111.36
1	e	134	LEU	N-CA-C	5.85	117.45	111.14
1	p	143	LYS	N-CA-C	5.84	117.45	111.14
1	o	100	ARG	N-CA-C	5.84	117.45	111.14
1	F	22	ILE	CB-CA-C	-5.83	104.50	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	143	LYS	N-CA-C	5.81	117.69	111.36
1	L	100	ARG	N-CA-C	5.80	117.40	111.14
1	R	145	GLY	N-CA-C	-5.79	104.42	112.18
1	R	106	VAL	N-CA-C	-5.77	104.73	110.62
1	r	142	ASP	N-CA-C	5.77	117.37	111.14
1	R	144	LEU	N-CA-C	5.76	117.64	111.36
1	M	93	ILE	CA-C-N	5.76	128.00	120.28
1	M	93	ILE	C-N-CA	5.76	128.00	120.28
1	l	23	ASN	N-CA-C	5.75	117.23	111.07
1	V	146	GLU	N-CA-C	5.73	117.52	111.28
1	L	72	GLN	N-CA-C	5.72	117.59	111.36
1	v	143	LYS	N-CA-C	5.71	117.31	111.14
1	Q	72	GLN	N-CA-C	5.71	117.58	111.36
1	C	146	GLU	N-CA-C	5.70	117.58	111.36
1	w	64	LEU	N-CA-C	-5.69	105.07	111.28
1	c	145	GLY	N-CA-C	-5.69	105.59	112.48
1	R	22	ILE	N-CA-C	-5.68	104.96	110.42
1	w	45	ARG	NE-CZ-NH2	5.67	124.31	119.20
1	D	23	ASN	N-CA-C	5.66	117.25	111.14
1	U	39	GLU	N-CA-C	5.65	117.25	111.14
1	h	146	GLU	N-CA-C	5.64	117.11	111.07
1	I	158	PRO	CA-C-N	5.64	131.84	121.70
1	I	158	PRO	C-N-CA	5.64	131.84	121.70
1	m	145	GLY	N-CA-C	-5.64	104.33	111.72
1	a	3	GLY	N-CA-C	5.60	120.22	112.37
1	N	120	LEU	N-CA-C	5.60	117.46	111.36
1	l	72	GLN	N-CA-C	5.59	117.45	111.36
1	B	81	GLN	N-CA-C	5.58	120.21	113.17
1	G	64	LEU	N-CA-C	-5.58	105.20	111.28
1	d	91	LEU	N-CA-C	-5.57	105.31	111.71
1	X	145	GLY	N-CA-C	-5.56	104.72	112.18
1	D	100	ARG	N-CA-C	5.56	117.15	111.14
1	q	97	VAL	CB-CA-C	-5.56	104.86	111.97
1	E	51	GLU	CB-CG-CD	5.56	122.05	112.60
1	f	126	ASP	O-C-N	-5.55	116.23	122.12
1	b	142	ASP	N-CA-C	5.55	117.14	111.14
1	F	72	GLN	N-CA-C	5.54	117.13	111.14
1	R	63	LEU	N-CA-C	5.53	118.24	111.82
1	D	121	GLU	N-CA-C	-5.52	105.26	111.28
1	f	62	ILE	CB-CA-C	-5.51	104.70	112.14
1	O	22	ILE	CB-CA-C	-5.51	104.92	111.97
1	u	120	LEU	N-CA-C	5.51	117.28	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	105	ILE	N-CA-C	5.50	115.70	110.42
1	M	81	GLN	N-CA-C	5.47	119.65	112.92
1	J	110	GLU	N-CA-C	-5.47	105.32	111.28
1	W	101	LEU	N-CA-C	5.47	118.16	111.82
1	s	51	GLU	CA-C-N	5.47	127.61	120.28
1	s	51	GLU	C-N-CA	5.47	127.61	120.28
1	F	107	MET	N-CA-C	5.46	116.92	111.07
1	e	34	ASN	N-CA-C	5.46	117.31	111.36
1	c	115	THR	O-C-N	-5.45	116.34	122.12
1	c	144	LEU	N-CA-C	5.45	120.20	113.50
1	i	101	LEU	N-CA-C	5.45	118.14	111.82
1	r	38	THR	N-CA-C	5.45	117.22	111.28
1	X	100	ARG	N-CA-C	5.45	117.02	111.14
1	q	94	GLU	CA-C-N	5.44	127.57	120.28
1	q	94	GLU	C-N-CA	5.44	127.57	120.28
1	e	16	THR	N-CA-C	-5.43	105.36	111.28
1	V	51	GLU	CG-CD-OE2	5.43	130.90	118.40
1	l	146	GLU	N-CA-C	5.42	117.19	111.28
1	x	73	ARG	N-CA-C	5.42	118.30	110.28
1	c	22	ILE	CB-CA-C	-5.42	104.83	112.14
1	H	93	ILE	N-CA-C	5.41	116.13	110.62
1	x	143	LYS	N-CA-C	5.40	117.17	111.28
1	v	93	ILE	N-CA-C	5.39	116.12	110.62
1	O	2	GLN	N-CA-C	5.38	118.23	109.24
1	e	143	LYS	N-CA-C	5.38	116.83	111.07
1	n	111	LYS	N-CA-C	-5.38	106.70	113.20
1	I	100	ARG	N-CA-C	5.37	116.94	111.14
1	S	127	GLU	N-CA-CB	5.37	118.01	110.12
1	C	52	MET	N-CA-C	-5.37	105.43	111.28
1	D	58	ILE	CB-CA-C	-5.37	104.89	112.14
1	F	114	THR	N-CA-C	5.37	117.13	111.28
1	K	100	ARG	N-CA-C	5.37	116.94	111.14
1	b	23	ASN	N-CA-C	5.37	116.81	111.07
1	Q	2	GLN	N-CA-C	5.37	117.83	108.76
1	d	93	ILE	CB-CA-C	5.35	119.36	112.14
1	K	43	HIS	N-CA-C	5.34	117.18	111.36
1	J	23	ASN	N-CA-C	5.34	116.78	111.07
1	h	17	SER	O-C-N	5.34	127.57	122.07
1	S	51	GLU	CG-CD-OE2	5.33	130.66	118.40
1	d	26	PHE	N-CA-C	5.33	116.77	111.07
1	v	154	VAL	CB-CA-C	-5.32	104.46	111.70
1	R	143	LYS	CA-C-N	5.32	127.84	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	143	LYS	C-N-CA	5.32	127.84	120.29
1	f	2	GLN	N-CA-C	5.31	118.09	109.06
1	q	34	ASN	N-CA-C	5.31	117.98	111.82
1	O	122	LYS	N-CA-C	5.30	117.14	111.36
1	B	125	ALA	N-CA-C	5.30	116.75	111.07
1	P	112	GLN	N-CA-C	5.29	118.88	111.74
1	w	13	GLU	N-CA-C	-5.29	105.51	111.28
1	N	101	LEU	N-CA-C	5.29	117.79	111.71
1	U	125	ALA	CA-C-N	5.29	127.32	120.44
1	U	125	ALA	C-N-CA	5.29	127.32	120.44
1	j	3	GLY	N-CA-C	5.29	118.96	112.14
1	B	35	TRP	N-CA-C	-5.28	106.81	113.20
1	J	50	ASP	N-CA-CB	5.27	117.95	110.16
1	c	134	LEU	N-CA-C	5.26	116.70	111.07
1	j	73	ARG	N-CA-C	5.26	118.13	109.76
1	m	25	TYR	O-C-N	5.26	127.77	122.09
1	g	45	ARG	N-CA-C	-5.26	105.44	111.07
1	N	99	ASN	N-CA-C	5.26	117.09	111.36
1	W	124	VAL	N-CA-C	-5.26	105.37	110.42
1	G	120	LEU	N-CA-C	5.25	117.08	111.36
1	N	146	GLU	N-CA-C	5.24	116.67	111.07
1	j	134	LEU	N-CA-C	5.24	117.07	111.36
1	k	144	LEU	N-CA-C	5.24	117.07	111.36
1	w	93	ILE	CB-CA-C	5.24	119.21	112.14
1	j	143	LYS	N-CA-C	5.23	117.06	111.36
1	q	153	CYS	N-CA-C	5.22	119.80	113.38
1	D	99	ASN	CA-C-N	5.21	127.53	120.44
1	D	99	ASN	C-N-CA	5.21	127.53	120.44
1	t	33	ASP	CA-C-N	5.21	127.27	120.28
1	t	33	ASP	C-N-CA	5.21	127.27	120.28
1	G	71	TYR	CA-C-N	5.21	127.69	120.29
1	G	71	TYR	C-N-CA	5.21	127.69	120.29
1	a	109	ARG	N-CA-C	5.21	117.04	111.36
1	e	76	SER	N-CA-C	5.21	116.74	108.67
1	U	101	LEU	N-CA-C	5.20	117.85	111.82
1	k	101	LEU	N-CA-C	5.20	117.85	111.82
1	w	23	ASN	N-CA-C	5.20	116.63	111.07
1	X	114	THR	N-CA-C	5.19	116.94	111.28
1	p	2	GLN	N-CA-C	5.19	117.91	109.24
1	H	97	VAL	N-CA-C	5.18	115.39	110.42
1	W	68	LEU	CB-CA-C	-5.18	105.78	110.44
1	L	101	LEU	N-CA-C	5.17	117.00	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	100	ARG	N-CA-C	5.17	116.73	111.14
1	X	143	LYS	N-CA-C	5.17	117.00	111.36
1	x	117	ALA	N-CA-C	5.17	116.61	111.07
1	g	38	THR	N-CA-C	5.17	116.92	111.28
1	E	2	GLN	N-CA-C	5.16	116.79	108.32
1	O	94	GLU	N-CA-C	5.15	116.90	111.28
1	H	94	GLU	N-CA-C	5.14	116.88	111.28
1	D	143	LYS	N-CA-C	5.13	116.56	111.07
1	W	20	THR	N-CA-C	-5.13	105.69	111.28
1	h	18	GLU	CA-C-N	5.13	127.16	120.28
1	h	18	GLU	C-N-CA	5.13	127.16	120.28
1	b	85	GLU	N-CA-C	5.13	116.95	111.36
1	W	79	ILE	N-CA-C	5.13	115.15	107.51
1	h	101	LEU	N-CA-C	5.12	117.60	111.71
1	L	2	GLN	N-CA-C	5.12	116.38	107.93
1	X	146	GLU	N-CA-C	5.12	116.86	111.28
1	e	43	HIS	N-CA-C	5.12	116.55	111.07
1	a	101	LEU	N-CA-C	5.11	116.85	111.28
1	T	62	ILE	N-CA-C	5.11	115.83	110.62
1	H	146	GLU	N-CA-C	5.11	116.84	111.28
1	U	143	LYS	N-CA-C	5.10	116.92	111.36
1	U	94	GLU	N-CA-C	5.09	116.52	111.07
1	l	144	LEU	N-CA-C	5.09	116.91	111.36
1	L	23	ASN	N-CA-C	5.09	116.64	111.14
1	k	100	ARG	N-CA-C	5.09	116.64	111.14
1	T	3	GLY	N-CA-C	5.08	118.70	112.14
1	m	54	HIS	CB-CA-C	-5.07	102.92	110.88
1	a	23	ASN	N-CA-C	5.07	116.49	111.07
1	w	22	ILE	CB-CA-C	-5.06	105.49	111.97
1	u	51	GLU	CB-CG-CD	5.06	121.20	112.60
1	D	79	ILE	CB-CA-C	-5.05	104.06	110.98
1	I	143	LYS	N-CA-C	5.05	116.79	111.28
1	A	3	GLY	N-CA-C	5.05	118.66	112.14
1	f	38	THR	N-CA-C	5.05	116.78	111.28
1	G	35	TRP	N-CA-C	-5.04	106.90	113.16
1	H	23	ASN	N-CA-C	5.04	116.47	111.07
1	a	51	GLU	CG-CD-OE1	-5.04	106.80	118.40
1	o	66	ASP	CA-C-N	5.04	127.49	122.30
1	o	66	ASP	C-N-CA	5.04	127.49	122.30
1	E	51	GLU	CG-CD-OE1	-5.04	106.81	118.40
1	u	12	ASN	N-CA-C	5.04	116.77	111.28
1	X	149	TYR	CA-C-N	5.03	127.53	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	149	TYR	C-N-CA	5.03	127.53	120.28
1	x	146	GLU	N-CA-C	5.03	116.76	111.28
1	N	38	THR	N-CA-C	5.03	116.84	111.36
1	m	112	GLN	N-CA-C	5.03	118.66	111.92
1	t	120	LEU	N-CA-C	5.02	117.65	111.82
1	m	30	LYS	CA-C-N	5.01	127.41	120.29
1	m	30	LYS	C-N-CA	5.01	127.41	120.29
1	n	93	ILE	N-CA-C	5.01	115.73	110.62
1	H	108	CYS	CA-C-N	5.01	127.41	120.29
1	H	108	CYS	C-N-CA	5.01	127.41	120.29
1	R	142	ASP	N-CA-C	5.01	116.82	111.36
1	u	101	LEU	N-CA-C	5.01	117.47	111.71
1	F	4	ASP	CA-C-N	5.01	124.61	119.05
1	F	4	ASP	C-N-CA	5.01	124.61	119.05
1	p	80	GLY	N-CA-C	5.01	118.35	111.54
1	D	68	LEU	CB-CA-C	-5.00	104.39	110.15
1	A	93	ILE	N-CA-C	5.00	115.72	110.62
1	C	112	GLN	N-CA-C	5.00	118.64	112.24
1	U	7	VAL	CB-CA-C	-5.00	105.57	111.97
1	i	80	GLY	N-CA-C	5.00	119.49	111.64
1	n	51	GLU	CG-CD-OE1	5.00	129.90	118.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	q	94	GLU	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1285	0	1260	37	0
1	B	1285	0	1260	31	0
1	C	1285	0	1260	49	0
1	D	1285	0	1260	42	0
1	E	1285	0	1260	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1285	0	1260	33	0
1	G	1285	0	1260	49	0
1	H	1285	0	1260	35	0
1	I	1285	0	1260	32	0
1	J	1285	0	1260	26	0
1	K	1285	0	1260	36	0
1	L	1285	0	1260	36	0
1	M	1285	0	1260	55	0
1	N	1285	0	1260	20	0
1	O	1285	0	1260	33	0
1	P	1285	0	1260	34	0
1	Q	1285	0	1260	52	0
1	R	1285	0	1260	30	0
1	S	1285	0	1260	33	0
1	T	1285	0	1260	28	0
1	U	1285	0	1260	30	0
1	V	1285	0	1260	31	0
1	W	1285	0	1260	37	0
1	X	1285	0	1260	29	0
1	a	1285	0	1260	27	0
1	b	1285	0	1260	34	0
1	c	1285	0	1260	30	0
1	d	1285	0	1260	32	0
1	e	1285	0	1260	52	0
1	f	1285	0	1260	37	0
1	g	1285	0	1260	20	0
1	h	1285	0	1260	35	0
1	i	1285	0	1259	34	0
1	j	1285	0	1260	16	0
1	k	1285	0	1260	44	0
1	l	1285	0	1260	31	0
1	m	1281	0	1256	31	0
1	n	1285	0	1260	26	0
1	o	1285	0	1260	51	0
1	p	1281	0	1256	40	0
1	q	1285	0	1260	52	0
1	r	1285	0	1260	31	0
1	s	1285	0	1260	32	0
1	t	1285	0	1260	50	0
1	u	1285	0	1260	28	0
1	v	1285	0	1260	21	0
1	w	1285	0	1260	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	x	1285	0	1260	42	0
2	B	43	0	30	8	0
2	C	43	0	30	23	0
2	F	43	0	30	4	0
2	H	43	0	30	7	0
2	I	43	0	30	5	0
2	L	43	0	30	12	0
2	M	43	0	30	8	0
2	P	43	0	30	9	0
2	R	43	0	30	14	0
2	S	43	0	30	5	0
2	U	43	0	30	4	0
2	X	43	0	30	6	0
2	a	43	0	30	5	0
2	c	43	0	30	6	0
2	e	43	0	30	9	0
2	g	43	0	30	11	0
2	j	43	0	30	6	0
2	k	43	0	30	12	0
2	n	43	0	30	6	0
2	o	43	0	30	8	0
2	q	43	0	30	16	0
2	t	43	0	30	13	0
2	v	43	0	30	3	0
2	x	43	0	30	9	0
3	A	131	0	0	7	0
3	B	120	0	0	2	0
3	C	89	0	0	16	0
3	D	105	0	0	11	0
3	E	104	0	0	12	0
3	F	102	0	0	3	0
3	G	115	0	0	10	0
3	H	135	0	0	13	0
3	I	127	0	0	9	0
3	J	142	0	0	6	0
3	K	115	0	0	7	0
3	L	116	0	0	17	0
3	M	115	0	0	9	0
3	N	122	0	0	3	0
3	O	127	0	0	6	0
3	P	127	0	0	3	0
3	Q	108	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	104	0	0	11	0
3	S	73	0	0	3	0
3	T	136	0	0	9	0
3	U	151	0	0	7	0
3	V	119	0	0	11	0
3	W	91	0	0	8	0
3	X	131	0	0	13	0
3	a	65	0	0	4	0
3	b	59	0	0	8	0
3	c	94	0	0	4	0
3	d	57	0	0	3	0
3	e	103	0	0	10	0
3	f	105	0	0	8	0
3	g	59	0	0	4	0
3	h	63	0	0	14	0
3	i	128	0	0	13	0
3	j	74	0	0	1	0
3	k	102	0	0	5	0
3	l	120	0	0	7	0
3	m	58	0	0	3	0
3	n	41	0	0	3	0
3	o	106	0	0	16	0
3	p	69	0	0	9	0
3	q	91	0	0	8	0
3	r	96	0	0	10	0
3	s	65	0	0	6	0
3	t	69	0	0	2	0
3	u	131	0	0	5	0
3	v	74	0	0	2	0
3	w	100	0	0	12	0
3	x	122	0	0	4	0
All	All	67560	0	61191	1703	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (1703) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:98:LEU:HB2	3:c:356:HOH:O	1.30	1.32
1:I:76:SER:HB2	3:I:320:HOH:O	1.39	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:73:ARG:HD3	3:W:217:HOH:O	1.38	1.23
1:X:74:ILE:HA	3:X:403:HOH:O	1.39	1.19
2:g:200:HEM:HBB2	2:g:200:HEM:HHC	1.24	1.18
1:o:14:GLN:HA	3:o:362:HOH:O	1.43	1.18
1:F:78:ARG:HD3	3:F:309:HOH:O	1.40	1.16
1:H:53:ARG:HA	3:H:373:HOH:O	1.45	1.13
2:j:200:HEM:HHC	2:j:200:HEM:HBB2	1.26	1.12
2:H:200:HEM:HHC	2:H:200:HEM:HBB2	1.27	1.10
1:b:61:ARG:HB3	3:b:252:HOH:O	1.50	1.10
1:X:129:GLU:HG2	3:X:334:HOH:O	1.51	1.10
1:S:107:MET:HE1	1:S:111:LYS:HG3	1.29	1.09
1:M:38:THR:HG21	1:M:159:THR:HG23	1.27	1.08
2:o:200:HEM:HBA2	3:o:321:HOH:O	1.51	1.08
1:e:140:LEU:HD12	3:e:375:HOH:O	1.50	1.07
1:V:159:THR:HG21	3:V:250:HOH:O	1.52	1.07
1:I:19:LEU:HD13	3:J:317:HOH:O	1.53	1.07
1:M:1:MET:HA	3:M:412:HOH:O	1.53	1.07
2:k:200:HEM:HBC2	2:k:200:HEM:HHH	1.29	1.07
1:X:78:ARG:NH1	1:X:92:ALA:HB1	1.69	1.07
2:L:200:HEM:HHC	2:L:200:HEM:HBB2	1.34	1.06
1:b:120:LEU:HD12	3:b:235:HOH:O	1.54	1.06
1:f:44:THR:HG21	3:f:272:HOH:O	1.56	1.05
2:e:200:HEM:HHC	2:e:200:HEM:HBB2	1.37	1.05
1:T:94:GLU:HG2	3:T:282:HOH:O	1.56	1.04
1:W:27:LEU:HD23	1:W:79:ILE:HD12	1.39	1.04
2:L:200:HEM:HBA1	3:L:373:HOH:O	1.57	1.03
1:a:15:LEU:C	1:a:15:LEU:HD23	1.84	1.03
1:D:88:GLU:HG2	3:D:216:HOH:O	1.58	1.01
1:t:156:ARG:HH22	1:x:152:GLN:NE2	1.58	0.99
2:X:200:HEM:HHC	2:X:200:HEM:HBB2	1.44	0.99
1:q:18:GLU:OE1	1:q:51:GLU:HG3	1.62	0.99
1:L:116:SER:HB2	3:L:368:HOH:O	1.62	0.99
2:P:200:HEM:HHC	2:P:200:HEM:HBB2	1.43	0.99
1:e:87:PHE:HE2	1:e:141:MET:HE3	1.28	0.99
1:w:48:SER:HB2	3:w:265:HOH:O	1.61	0.99
1:E:94:GLU:HG3	3:E:254:HOH:O	1.62	0.98
1:t:84:ARG:HB2	1:t:141:MET:HE1	1.42	0.98
1:A:28:HIS:HB3	3:A:326:HOH:O	1.64	0.97
1:i:156:ARG:HH22	1:p:152:GLN:HE22	1.12	0.97
1:j:156:ARG:HH22	1:u:152:GLN:HE22	1.10	0.97
1:S:79:ILE:HG22	3:S:338:HOH:O	1.63	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:33:ASP:OD1	1:F:38:THR:HG22	1.65	0.95
2:a:200:HEM:HHC	2:a:200:HEM:HBB2	1.45	0.95
2:C:200:HEM:HBA2	2:C:200:HEM:CMA	1.93	0.94
1:t:9:ARG:HH11	1:t:9:ARG:HG2	1.33	0.94
2:B:200:HEM:HBC2	2:B:200:HEM:HHD	1.49	0.93
1:H:61:ARG:NH2	1:H:115:THR:HB	1.82	0.93
1:h:69:PRO:HD3	3:h:260:HOH:O	1.65	0.93
1:o:56:GLU:HG3	1:p:26:PHE:HZ	1.31	0.93
1:b:86:GLN:HB3	3:b:244:HOH:O	1.68	0.93
1:u:156:ARG:HE	1:x:156:ARG:HH12	1.05	0.93
1:L:39:GLU:HB2	3:L:399:HOH:O	1.67	0.92
1:o:156:ARG:HD2	3:o:367:HOH:O	1.70	0.92
1:S:107:MET:HE3	1:S:111:LYS:HG2	1.50	0.91
1:r:117:ALA:O	1:r:121:GLU:HG3	1.69	0.91
1:S:107:MET:CE	1:S:111:LYS:CG	2.48	0.91
2:t:200:HEM:HHD	2:t:200:HEM:HBC2	1.51	0.91
1:q:34:ASN:HB3	3:q:387:HOH:O	1.71	0.91
1:S:107:MET:CE	1:S:111:LYS:HG3	2.00	0.91
1:Q:94:GLU:OE1	1:Q:127:GLU:HG3	1.70	0.90
1:x:27:LEU:HD23	1:x:79:ILE:HD12	1.52	0.90
1:d:152:GLN:HE22	1:o:156:ARG:HH22	1.16	0.90
1:W:1:MET:HE3	1:W:64:LEU:CD2	2.01	0.90
1:k:26:PHE:CZ	2:k:200:HEM:HBC1	2.07	0.90
1:x:140:LEU:HD12	3:x:415:HOH:O	1.71	0.90
1:q:53:ARG:HD2	3:q:379:HOH:O	1.71	0.90
1:k:26:PHE:CZ	2:k:200:HEM:CBC	2.54	0.89
1:w:98:LEU:O	1:w:102:LYS:HG3	1.72	0.89
2:k:200:HEM:HHC	2:k:200:HEM:HBB2	1.53	0.89
1:U:9:ARG:HG2	3:U:450:HOH:O	1.74	0.88
1:O:123:ILE:O	1:O:127:GLU:HG2	1.72	0.88
2:q:200:HEM:CGA	3:r:264:HOH:O	2.21	0.88
1:A:158:PRO:HB2	1:M:137:GLN:HE22	1.38	0.88
1:c:1:MET:HA	3:r:260:HOH:O	1.73	0.87
2:g:200:HEM:HBC2	2:g:200:HEM:HHD	1.57	0.87
1:t:156:ARG:HH22	1:x:152:GLN:HE22	0.88	0.87
1:W:1:MET:HE3	1:W:64:LEU:HD21	1.56	0.87
1:o:93:ILE:HG13	3:o:370:HOH:O	1.75	0.87
1:E:134:LEU:HD12	3:E:254:HOH:O	1.73	0.86
1:E:134:LEU:CD1	3:E:254:HOH:O	2.21	0.86
2:R:200:HEM:HMD2	2:R:200:HEM:HBD1	1.57	0.86
1:V:94:GLU:OE1	1:V:127:GLU:HB3	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:73:ARG:HD3	3:L:387:HOH:O	1.74	0.86
1:Q:38:THR:CG2	1:Q:159:THR:HG23	2.05	0.86
1:M:38:THR:CG2	1:M:159:THR:HG23	2.04	0.86
1:f:2:GLN:HG2	3:f:277:HOH:O	1.75	0.86
1:S:33:ASP:OD1	1:S:38:THR:HG22	1.76	0.86
2:M:200:HEM:HMC2	2:M:200:HEM:HBC2	1.56	0.86
1:H:56:GLU:HB3	3:H:373:HOH:O	1.76	0.85
1:a:123:ILE:O	1:a:127:GLU:HG2	1.77	0.85
1:G:38:THR:CG2	1:G:159:THR:HG23	2.07	0.85
1:A:33:ASP:OD1	1:A:38:THR:HG22	1.75	0.85
1:C:2:GLN:HG3	3:C:325:HOH:O	1.76	0.85
3:U:352:HOH:O	1:X:156:ARG:HD3	1.75	0.85
1:S:107:MET:HE1	1:S:111:LYS:CG	2.06	0.84
1:q:1:MET:HE3	1:q:64:LEU:HD21	1.59	0.84
1:A:1:MET:HE3	1:A:64:LEU:HD23	1.59	0.84
1:o:138:LEU:HD23	1:o:141:MET:HE2	1.58	0.84
1:I:93:ILE:HB	3:I:384:HOH:O	1.78	0.83
1:Q:84:ARG:HD3	3:Q:302:HOH:O	1.78	0.83
1:t:156:ARG:NH2	1:x:152:GLN:HE22	1.74	0.83
1:o:56:GLU:HG3	1:p:26:PHE:CZ	2.13	0.83
2:S:200:HEM:HMB1	2:S:200:HEM:HBB2	1.58	0.83
1:W:22:ILE:HG23	3:W:287:HOH:O	1.78	0.83
1:w:159:THR:HA	3:w:219:HOH:O	1.78	0.83
1:B:18:GLU:HG3	1:B:51:GLU:HG3	1.60	0.82
1:Q:88:GLU:HG2	3:Q:260:HOH:O	1.80	0.82
1:c:25:TYR:HE2	3:c:389:HOH:O	1.63	0.82
1:E:102:LYS:HG2	3:R:401:HOH:O	1.79	0.81
1:o:100:ARG:CZ	3:o:362:HOH:O	2.28	0.81
3:L:399:HOH:O	1:P:157:PRO:HB3	1.78	0.81
2:c:200:HEM:HHC	2:c:200:HEM:HBB2	1.62	0.81
1:a:30:LYS:HE2	1:b:56:GLU:HG3	1.61	0.81
1:e:87:PHE:CE2	1:e:141:MET:HE3	2.14	0.81
2:H:200:HEM:HBB2	2:H:200:HEM:CHC	2.00	0.80
1:k:26:PHE:CE2	2:k:200:HEM:HBC1	2.16	0.80
1:d:152:GLN:NE2	1:o:156:ARG:HH22	1.80	0.80
1:c:25:TYR:CE2	3:c:389:HOH:O	2.34	0.80
1:p:53:ARG:HG2	3:p:212:HOH:O	1.81	0.80
1:G:159:THR:HG22	3:G:232:HOH:O	1.81	0.80
1:Q:88:GLU:CG	3:Q:260:HOH:O	2.29	0.80
1:k:123:ILE:O	1:k:127:GLU:HG2	1.82	0.80
2:X:200:HEM:HAD1	3:X:304:HOH:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:LEU:HB2	3:D:287:HOH:O	1.82	0.79
1:s:159:THR:CG2	3:s:201:HOH:O	2.30	0.79
1:h:68:LEU:HA	3:h:260:HOH:O	1.80	0.79
2:B:200:HEM:HBC2	2:B:200:HEM:CHD	2.09	0.79
1:G:102:LYS:HB2	1:G:103:PRO:CD	2.13	0.79
2:q:200:HEM:HBC2	2:q:200:HEM:HMC2	1.63	0.79
1:U:32:GLN:HE21	1:U:86:GLN:NE2	1.79	0.79
2:L:200:HEM:HHC	2:L:200:HEM:CBB	2.14	0.78
1:E:123:ILE:O	1:E:127:GLU:HG2	1.83	0.78
1:e:156:ARG:HD2	3:e:318:HOH:O	1.83	0.78
2:g:200:HEM:HHC	2:g:200:HEM:CBB	2.08	0.78
1:j:156:ARG:HH22	1:u:152:GLN:NE2	1.81	0.78
1:C:86:GLN:HB2	3:C:380:HOH:O	1.84	0.78
1:S:107:MET:CE	1:S:111:LYS:HG2	2.11	0.78
1:n:39:GLU:OE2	1:n:155:SER:HB3	1.84	0.78
1:o:9:ARG:HD3	3:o:404:HOH:O	1.82	0.78
1:t:24:GLN:NE2	1:t:78:ARG:H	1.81	0.78
1:J:4:ASP:HB2	3:J:220:HOH:O	1.83	0.77
1:O:87:PHE:HE2	1:O:141:MET:HE3	1.48	0.77
1:Q:27:LEU:HD21	3:R:327:HOH:O	1.84	0.77
2:k:200:HEM:HBC2	2:k:200:HEM:CHD	2.03	0.77
1:e:93:ILE:HD11	3:e:387:HOH:O	1.84	0.77
2:I:200:HEM:HBC2	2:I:200:HEM:HHD	1.67	0.76
1:E:146:GLU:HB3	3:E:223:HOH:O	1.86	0.76
1:q:18:GLU:OE1	1:q:51:GLU:CG	2.33	0.76
1:P:147:GLU:HB2	3:P:422:HOH:O	1.83	0.76
1:V:61:ARG:NH2	1:V:115:THR:HB	2.01	0.76
1:E:102:LYS:HB2	1:E:103:PRO:HD2	1.68	0.76
1:K:28:HIS:O	1:K:32:GLN:HG3	1.86	0.76
1:l:2:GLN:HG3	3:l:203:HOH:O	1.85	0.76
1:C:1:MET:HA	3:C:348:HOH:O	1.85	0.76
2:C:200:HEM:FE	2:C:200:HEM:ND	1.53	0.75
1:a:15:LEU:C	1:a:15:LEU:CD2	2.60	0.75
1:c:94:GLU:OE2	1:c:127:GLU:HB3	1.86	0.75
1:f:32:GLN:CD	3:f:272:HOH:O	2.30	0.75
1:M:64:LEU:O	1:M:64:LEU:HD23	1.87	0.75
1:D:123:ILE:O	1:D:127:GLU:HG2	1.87	0.75
1:G:97:VAL:HG23	3:G:286:HOH:O	1.86	0.75
1:Q:70:ASN:HB3	3:Q:303:HOH:O	1.87	0.75
1:o:100:ARG:NH2	3:o:362:HOH:O	2.20	0.75
1:G:38:THR:HG21	1:G:159:THR:HG23	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:200:HEM:O1D	1:V:53:ARG:NH1	2.20	0.75
1:w:53:ARG:O	1:w:57:GLU:HG3	1.87	0.75
1:N:78:ARG:HB2	3:N:319:HOH:O	1.87	0.74
3:U:352:HOH:O	1:X:156:ARG:CD	2.35	0.74
1:M:53:ARG:HG2	3:M:415:HOH:O	1.87	0.74
1:A:94:GLU:OE2	1:A:134:LEU:CD1	2.35	0.74
1:O:117:ALA:O	1:O:121:GLU:HG3	1.87	0.74
1:l:143:LYS:HE3	3:p:253:HOH:O	1.86	0.74
1:U:4:ASP:HB3	1:U:7:VAL:CG2	2.18	0.74
1:h:93:ILE:HG13	3:h:224:HOH:O	1.86	0.74
1:k:50:ASP:OD2	1:k:53:ARG:NH2	2.21	0.74
1:D:33:ASP:OD1	1:D:38:THR:HG22	1.87	0.74
1:x:50:ASP:OD2	1:x:53:ARG:NH2	2.21	0.74
1:G:159:THR:CG2	3:G:232:HOH:O	2.36	0.74
2:a:200:HEM:HBC2	2:a:200:HEM:CMC	2.18	0.74
1:b:4:ASP:HB3	1:b:7:VAL:HG23	1.69	0.74
1:a:15:LEU:HD23	1:a:15:LEU:O	1.87	0.73
1:b:50:ASP:OD2	1:b:53:ARG:NH2	2.21	0.73
1:C:106:VAL:HA	3:C:364:HOH:O	1.89	0.73
1:G:110:GLU:HG3	3:G:269:HOH:O	1.88	0.73
1:q:52:MET:HG2	2:q:200:HEM:NC	2.03	0.73
1:d:137:GLN:NE2	1:d:149:TYR:OH	2.20	0.73
1:m:49:PHE:HD2	2:n:200:HEM:HBD2	1.54	0.73
1:q:1:MET:HE3	1:q:64:LEU:CD2	2.18	0.73
1:D:93:ILE:HB	3:D:245:HOH:O	1.88	0.73
1:l:102:LYS:HB2	1:l:103:PRO:HD2	1.69	0.73
1:q:52:MET:HG2	2:q:200:HEM:C4C	2.24	0.73
1:u:122:LYS:HD3	3:u:208:HOH:O	1.88	0.73
1:S:107:MET:HE3	1:S:111:LYS:CG	2.17	0.73
1:X:129:GLU:CG	3:X:334:HOH:O	2.20	0.73
1:Q:15:LEU:HD23	3:Q:303:HOH:O	1.89	0.72
1:k:26:PHE:CE1	2:k:200:HEM:CBC	2.72	0.72
1:n:74:ILE:HG22	3:n:320:HOH:O	1.88	0.72
1:Q:38:THR:HG23	1:Q:159:THR:HG23	1.71	0.72
1:W:94:GLU:OE1	1:W:130:HIS:ND1	2.19	0.72
1:s:159:THR:HG22	3:s:201:HOH:O	1.89	0.72
1:w:94:GLU:CG	3:w:288:HOH:O	2.36	0.72
1:s:38:THR:CG2	1:s:159:THR:HG23	2.20	0.72
1:S:81:GLN:HG2	3:S:338:HOH:O	1.90	0.72
1:m:50:ASP:OD2	1:m:53:ARG:NH2	2.21	0.72
1:G:28:HIS:CD2	1:G:86:GLN:HG2	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:50:ASP:OD2	1:L:53:ARG:NH2	2.23	0.72
3:l:243:HOH:O	1:p:159:THR:CG2	2.38	0.72
1:u:156:ARG:HE	1:x:156:ARG:NH1	1.85	0.72
1:h:38:THR:HG21	1:h:159:THR:HG23	1.72	0.72
1:Q:100:ARG:NH1	1:Q:100:ARG:HB2	2.05	0.72
2:R:200:HEM:HBD1	2:R:200:HEM:CMD	2.19	0.72
1:P:6:ASP:OD1	1:P:9:ARG:NH2	2.23	0.71
1:t:64:LEU:C	1:t:64:LEU:HD23	2.14	0.71
1:t:152:GLN:HE22	1:x:156:ARG:HH22	1.39	0.71
1:E:159:THR:HG23	3:E:255:HOH:O	1.90	0.71
1:G:4:ASP:HB3	1:G:7:VAL:HG23	1.71	0.71
1:l:50:ASP:OD1	1:l:53:ARG:NH2	2.22	0.71
1:c:64:LEU:O	1:c:64:LEU:HD23	1.91	0.71
1:m:49:PHE:CD2	2:n:200:HEM:HBD2	2.26	0.71
1:C:86:GLN:CB	3:C:380:HOH:O	2.39	0.71
2:L:200:HEM:HBC2	2:L:200:HEM:HHD	1.73	0.71
1:n:159:THR:HG21	3:n:305:HOH:O	1.89	0.71
1:q:53:ARG:NH1	2:q:200:HEM:O1D	2.23	0.71
1:t:9:ARG:HH11	1:t:9:ARG:CG	2.03	0.71
1:T:94:GLU:CG	3:T:282:HOH:O	2.27	0.71
1:L:73:ARG:HB2	3:L:387:HOH:O	1.90	0.71
1:A:32:GLN:NE2	3:A:326:HOH:O	2.24	0.71
1:b:4:ASP:HB3	1:b:7:VAL:CG2	2.20	0.71
2:k:200:HEM:HHD	2:k:200:HEM:CBC	2.09	0.71
1:O:68:LEU:HB3	3:O:322:HOH:O	1.90	0.70
1:X:78:ARG:NH1	1:X:92:ALA:CB	2.52	0.70
1:o:156:ARG:CD	3:o:367:HOH:O	2.30	0.70
1:W:53:ARG:NH1	3:W:265:HOH:O	2.23	0.70
1:a:9:ARG:NH1	3:a:362:HOH:O	2.24	0.70
1:r:100:ARG:NH1	3:r:295:HOH:O	2.25	0.70
1:Q:57:GLU:CD	3:Q:263:HOH:O	2.35	0.70
1:s:78:ARG:NH1	1:s:92:ALA:HB1	2.05	0.70
1:B:18:GLU:HG3	1:B:51:GLU:CG	2.21	0.70
1:C:123:ILE:O	1:C:127:GLU:HG2	1.91	0.70
1:H:1:MET:N	3:H:431:HOH:O	2.25	0.70
2:S:200:HEM:HBB2	2:S:200:HEM:CMB	2.20	0.70
2:o:200:HEM:O1D	1:p:53:ARG:NH1	2.25	0.70
1:w:70:ASN:ND2	3:w:300:HOH:O	2.23	0.70
1:L:40:LEU:N	3:L:399:HOH:O	2.25	0.70
1:b:86:GLN:CB	3:b:244:HOH:O	2.33	0.70
1:w:53:ARG:NH1	2:x:200:HEM:O2A	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ILE:HG21	3:C:378:HOH:O	1.91	0.70
1:N:94:GLU:OE2	1:N:127:GLU:HB3	1.91	0.70
1:U:53:ARG:NH1	2:U:200:HEM:O2A	2.24	0.70
1:k:74:ILE:HG12	1:k:75:GLY:N	2.04	0.70
1:w:94:GLU:HG3	3:w:288:HOH:O	1.91	0.70
1:x:137:GLN:HA	3:x:415:HOH:O	1.90	0.70
1:B:73:ARG:NH1	1:e:73:ARG:HD3	2.07	0.70
1:b:152:GLN:OE1	1:f:156:ARG:NH2	2.20	0.70
1:k:149:TYR:C	1:k:149:TYR:CD2	2.70	0.69
1:w:149:TYR:C	1:w:149:TYR:CD2	2.70	0.69
1:V:50:ASP:OD2	1:V:53:ARG:NH2	2.24	0.69
1:c:117:ALA:O	1:c:121:GLU:HG3	1.92	0.69
1:q:90:ASP:O	1:q:93:ILE:HG22	1.91	0.69
2:g:200:HEM:HBB2	2:g:200:HEM:CHC	2.06	0.69
1:L:100:ARG:HD3	3:L:380:HOH:O	1.91	0.69
1:e:97:VAL:CG1	1:e:101:LEU:HD12	2.23	0.69
1:i:123:ILE:O	1:i:127:GLU:HG2	1.92	0.69
1:E:84:ARG:NH2	3:E:287:HOH:O	2.26	0.69
1:c:123:ILE:O	1:c:127:GLU:HG2	1.92	0.69
1:s:38:THR:HG21	1:s:159:THR:HG23	1.73	0.69
1:W:70:ASN:HB2	3:W:257:HOH:O	1.91	0.69
1:i:79:ILE:HG22	3:i:295:HOH:O	1.92	0.69
1:q:24:GLN:NE2	1:q:78:ARG:H	1.91	0.69
2:t:200:HEM:HHC	2:t:200:HEM:HBB2	1.75	0.69
1:K:97:VAL:HG11	1:K:127:GLU:HG3	1.75	0.69
1:w:107:MET:SD	1:w:111:LYS:HE3	2.33	0.69
1:B:73:ARG:HH11	1:e:73:ARG:HD3	1.58	0.69
1:v:53:ARG:NH1	2:v:200:HEM:O1D	2.26	0.69
1:x:12:ASN:ND2	1:x:70:ASN:H	1.91	0.69
1:U:4:ASP:HB3	1:U:7:VAL:HG23	1.75	0.68
1:B:12:ASN:ND2	1:B:70:ASN:H	1.90	0.68
2:g:200:HEM:HBC1	1:h:26:PHE:CE2	2.27	0.68
1:E:141:MET:HG2	1:E:146:GLU:HG3	1.74	0.68
1:s:52:MET:HE2	2:t:200:HEM:NC	2.09	0.68
1:Q:38:THR:HG21	1:Q:159:THR:HG23	1.76	0.68
1:s:123:ILE:O	1:s:127:GLU:HG2	1.94	0.68
1:d:137:GLN:HE22	1:n:158:PRO:HB2	1.59	0.68
1:l:53:ARG:NH1	3:l:286:HOH:O	2.26	0.68
1:R:50:ASP:OD1	1:R:53:ARG:NH2	2.27	0.68
1:c:33:ASP:OD1	1:c:38:THR:HG22	1.94	0.68
1:o:100:ARG:NE	3:o:362:HOH:O	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:96:ASP:HB3	3:L:388:HOH:O	1.94	0.68
2:C:200:HEM:HBA2	2:C:200:HEM:HMA1	1.76	0.67
1:M:64:LEU:HD23	1:M:64:LEU:C	2.19	0.67
1:W:27:LEU:HD23	1:W:79:ILE:CD1	2.19	0.67
1:p:123:ILE:O	1:p:127:GLU:HG2	1.94	0.67
1:M:28:HIS:CD2	1:M:86:GLN:HG2	2.29	0.67
1:o:53:ARG:NE	3:o:327:HOH:O	2.21	0.67
1:A:74:ILE:HB	3:A:221:HOH:O	1.93	0.67
1:R:102:LYS:HB2	1:R:103:PRO:HD3	1.75	0.67
2:F:200:HEM:HBD1	3:F:323:HOH:O	1.95	0.67
2:R:200:HEM:HHC	2:R:200:HEM:HBB2	1.75	0.67
1:b:18:GLU:O	1:b:22:ILE:HG13	1.94	0.67
2:q:200:HEM:HBC2	2:q:200:HEM:CMC	2.25	0.67
1:x:12:ASN:HD21	1:x:69:PRO:HA	1.59	0.67
1:B:12:ASN:HD21	1:B:69:PRO:HA	1.60	0.67
1:K:18:GLU:OE1	1:K:51:GLU:CD	2.38	0.67
1:k:1:MET:HE3	1:k:64:LEU:CD2	2.24	0.67
1:m:117:ALA:O	1:m:121:GLU:HG3	1.95	0.66
1:u:50:ASP:OD1	1:u:53:ARG:NH2	2.28	0.66
1:X:53:ARG:HD3	2:X:200:HEM:O2D	1.96	0.66
1:t:9:ARG:HG2	1:t:9:ARG:NH1	2.07	0.66
1:A:22:ILE:HD11	1:A:52:MET:HA	1.77	0.66
1:U:129:GLU:CG	3:U:319:HOH:O	2.43	0.66
1:b:11:LEU:HD13	3:b:252:HOH:O	1.96	0.66
1:A:107:MET:O	1:A:111:LYS:HG2	1.96	0.66
1:D:61:ARG:NH2	1:D:115:THR:HB	2.11	0.66
3:T:325:HOH:O	1:V:1:MET:CE	2.43	0.66
1:i:156:ARG:HH22	1:p:152:GLN:NE2	1.91	0.66
1:x:82:THR:O	1:x:86:GLN:HG3	1.96	0.66
1:C:5:PRO:HD2	3:C:384:HOH:O	1.97	0.65
1:C:50:ASP:OD1	1:C:53:ARG:NH2	2.29	0.65
1:T:118:VAL:HG12	1:T:122:LYS:HE3	1.77	0.65
1:e:100:ARG:O	1:e:103:PRO:HD2	1.95	0.65
1:G:38:THR:HG23	1:G:159:THR:HG23	1.78	0.65
1:L:28:HIS:CD2	1:L:86:GLN:HG2	2.31	0.65
1:t:50:ASP:OD1	1:t:53:ARG:NH2	2.30	0.65
2:B:200:HEM:HHC	2:B:200:HEM:HBB2	1.76	0.65
1:t:123:ILE:O	1:t:127:GLU:HG2	1.96	0.65
1:e:14:GLN:O	1:e:17:SER:HB3	1.96	0.65
1:f:143:LYS:HB3	3:v:306:HOH:O	1.96	0.65
1:M:123:ILE:O	1:M:127:GLU:HG2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:200:HEM:HHC	2:j:200:HEM:CBB	2.13	0.65
2:B:200:HEM:HHD	2:B:200:HEM:CBC	2.23	0.65
1:A:1:MET:HE3	1:A:64:LEU:CD2	2.25	0.65
1:M:34:ASN:HB3	3:M:391:HOH:O	1.97	0.65
1:W:64:LEU:C	1:W:64:LEU:HD23	2.22	0.65
1:e:50:ASP:OD1	1:e:53:ARG:NH2	2.30	0.65
1:x:49:PHE:HD2	2:x:200:HEM:HBD2	1.61	0.65
1:W:1:MET:CE	1:W:64:LEU:HD21	2.26	0.65
2:C:200:HEM:CMA	2:C:200:HEM:CBA	2.73	0.64
1:K:50:ASP:OD1	1:K:53:ARG:NH2	2.30	0.64
1:M:9:ARG:HG3	1:M:9:ARG:HH11	1.60	0.64
1:s:52:MET:HE2	2:t:200:HEM:C1C	2.32	0.64
1:m:135:GLU:O	1:m:139:GLU:HG3	1.98	0.64
1:k:157:PRO:HD3	1:q:39:GLU:HB3	1.79	0.64
1:u:156:ARG:NE	1:x:156:ARG:HH12	1.86	0.64
2:o:200:HEM:HMD3	3:p:212:HOH:O	1.97	0.64
1:A:124:VAL:O	1:A:128:GLU:HG3	1.97	0.64
1:R:52:MET:HE1	2:R:200:HEM:C4C	2.33	0.64
1:H:159:THR:CB	3:H:422:HOH:O	2.45	0.64
1:q:62:ILE:HG22	1:q:69:PRO:HD3	1.80	0.64
1:D:93:ILE:HD13	3:D:245:HOH:O	1.97	0.64
1:F:124:VAL:O	1:F:128:GLU:HG3	1.98	0.63
1:u:64:LEU:HD23	1:u:65:LEU:HD23	1.80	0.63
1:A:40:LEU:HD13	3:A:294:HOH:O	1.96	0.63
1:H:56:GLU:CB	3:H:373:HOH:O	2.38	0.63
2:g:200:HEM:HBC2	2:g:200:HEM:CHD	2.22	0.63
1:s:50:ASP:OD2	1:s:53:ARG:NH2	2.30	0.63
1:P:50:ASP:OD2	1:P:53:ARG:NH2	2.31	0.63
1:V:123:ILE:O	1:V:127:GLU:HG2	1.98	0.63
1:v:74:ILE:HG12	1:v:75:GLY:N	2.12	0.63
3:T:325:HOH:O	1:V:1:MET:HE1	1.97	0.63
1:W:64:LEU:HD23	1:W:64:LEU:O	1.98	0.63
1:a:30:LYS:HE2	1:b:56:GLU:CG	2.28	0.63
1:q:2:GLN:NE2	3:q:367:HOH:O	2.21	0.63
1:x:119:LEU:C	1:x:119:LEU:HD12	2.24	0.63
1:F:53:ARG:NH1	2:F:200:HEM:O1A	2.32	0.63
1:n:19:LEU:HD22	2:n:200:HEM:HBB1	1.79	0.63
1:C:129:GLU:CG	3:C:312:HOH:O	2.45	0.63
2:H:200:HEM:HHC	2:H:200:HEM:CBB	2.17	0.63
1:W:28:HIS:O	1:W:32:GLN:HG3	1.99	0.63
1:k:87:PHE:CD2	1:k:141:MET:HE3	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:6:ASP:OD1	1:S:9:ARG:NH2	2.32	0.63
1:p:2:GLN:HG3	3:p:251:HOH:O	1.98	0.63
1:r:139:GLU:O	1:r:143:LYS:HG3	1.98	0.63
1:E:107:MET:SD	1:E:111:LYS:HE3	2.39	0.62
1:l:2:GLN:CG	3:l:203:HOH:O	2.46	0.62
1:u:102:LYS:NZ	3:u:324:HOH:O	2.28	0.62
2:C:200:HEM:HMB1	1:D:26:PHE:CZ	2.34	0.62
1:e:70:ASN:ND2	3:e:361:HOH:O	2.32	0.62
1:f:27:LEU:HD23	1:f:79:ILE:HD12	1.81	0.62
1:k:1:MET:CE	1:k:64:LEU:HD21	2.29	0.62
1:f:29:SER:HA	3:f:272:HOH:O	1.99	0.62
1:A:9:ARG:HB3	3:A:329:HOH:O	1.98	0.62
1:C:138:LEU:O	1:C:141:MET:HB2	1.99	0.62
1:m:51:GLU:OE2	1:m:54:HIS:ND1	2.32	0.62
1:o:84:ARG:HB2	1:o:141:MET:HE1	1.81	0.62
1:A:135:GLU:O	1:A:139:GLU:HG3	2.00	0.62
1:A:50:ASP:OD1	1:A:53:ARG:NH2	2.32	0.62
1:A:158:PRO:HB2	1:M:137:GLN:NE2	2.13	0.62
1:L:17:SER:HB2	1:L:100:ARG:NH2	2.15	0.62
1:O:50:ASP:OD1	1:O:53:ARG:NH2	2.30	0.62
1:B:52:MET:HE1	2:B:200:HEM:CHD	2.30	0.62
1:B:73:ARG:HH11	1:e:73:ARG:CD	2.10	0.62
1:J:147:GLU:CD	1:J:147:GLU:H	2.07	0.62
1:T:1:MET:N	3:T:218:HOH:O	2.28	0.62
1:e:4:ASP:OD2	1:e:6:ASP:HB2	2.00	0.62
1:o:138:LEU:CD2	1:o:141:MET:HE2	2.29	0.62
1:E:102:LYS:HB2	1:E:103:PRO:CD	2.29	0.62
1:P:1:MET:HE3	1:P:64:LEU:HD21	1.81	0.62
1:e:53:ARG:NH1	3:e:367:HOH:O	2.33	0.62
1:f:48:SER:O	1:f:52:MET:HG3	2.00	0.62
1:p:2:GLN:CG	3:p:251:HOH:O	2.48	0.62
1:A:153:CYS:SG	3:A:294:HOH:O	2.52	0.62
1:K:122:LYS:HG3	3:K:304:HOH:O	1.99	0.62
1:T:1:MET:HE3	3:T:315:HOH:O	2.00	0.61
1:b:97:VAL:HG11	1:b:127:GLU:HG3	1.81	0.61
1:G:4:ASP:HB3	1:G:7:VAL:CG2	2.30	0.61
1:P:1:MET:HE3	1:P:64:LEU:CD2	2.30	0.61
1:b:62:ILE:N	3:b:252:HOH:O	2.33	0.61
1:j:156:ARG:NH2	1:u:152:GLN:HE22	1.91	0.61
1:l:45:ARG:O	1:l:49:PHE:HD1	1.84	0.61
1:t:156:ARG:NH2	1:x:152:GLN:NE2	2.40	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:139:GLU:O	1:G:143:LYS:HG3	2.00	0.61
1:b:61:ARG:NH2	1:b:115:THR:HB	2.16	0.61
1:C:2:GLN:CG	3:C:325:HOH:O	2.41	0.61
2:x:200:HEM:CBB	2:x:200:HEM:HHC	2.29	0.61
1:i:22:ILE:HD11	1:i:52:MET:HA	1.81	0.61
1:I:50:ASP:OD1	1:I:53:ARG:NH2	2.34	0.61
1:I:52:MET:HB3	2:I:200:HEM:CHD	2.30	0.61
1:U:39:GLU:O	1:X:157:PRO:HG3	2.00	0.61
1:E:4:ASP:HB2	3:E:228:HOH:O	2.01	0.61
1:e:31:MET:HE1	1:e:80:GLY:O	2.01	0.61
1:k:10:LEU:HD21	1:k:104:GLY:HA3	1.83	0.61
1:D:64:LEU:C	1:D:64:LEU:HD23	2.25	0.61
1:H:153:CYS:SG	3:H:388:HOH:O	2.40	0.61
1:J:99:ASN:ND2	3:J:313:HOH:O	2.34	0.61
1:b:102:LYS:HB2	1:b:103:PRO:HD2	1.82	0.61
1:c:28:HIS:CD2	1:c:86:GLN:HG2	2.36	0.61
1:h:9:ARG:NE	3:h:202:HOH:O	2.34	0.61
1:I:82:THR:O	1:I:86:GLN:HG3	2.01	0.60
1:C:49:PHE:HZ	2:C:200:HEM:HAD1	1.67	0.60
1:H:78:ARG:NH1	1:H:92:ALA:HB1	2.16	0.60
1:b:101:LEU:HD22	1:b:120:LEU:HD13	1.83	0.60
1:h:22:ILE:HD11	1:h:52:MET:HA	1.83	0.60
1:l:119:LEU:O	1:l:119:LEU:HD12	2.01	0.60
2:C:200:HEM:HBA2	2:C:200:HEM:HMA3	1.82	0.60
1:L:108:CYS:HB3	3:L:368:HOH:O	2.01	0.60
2:M:200:HEM:HBC2	2:M:200:HEM:CMC	2.30	0.60
1:d:79:ILE:N	1:d:79:ILE:HD13	2.16	0.60
1:r:53:ARG:HG2	3:r:291:HOH:O	2.02	0.60
1:t:14:GLN:O	1:t:18:GLU:HG2	2.02	0.60
1:o:94:GLU:OE1	1:o:130:HIS:ND1	2.28	0.60
1:H:50:ASP:OD2	1:H:53:ARG:NH2	2.34	0.60
1:P:87:PHE:CE2	1:P:141:MET:HE3	2.36	0.60
1:U:129:GLU:HG2	3:U:319:HOH:O	2.02	0.60
1:c:149:TYR:C	1:c:149:TYR:CD2	2.78	0.60
1:J:87:PHE:HE2	1:J:141:MET:HE3	1.66	0.60
1:e:156:ARG:HH21	1:q:156:ARG:NH2	1.98	0.60
1:k:30:LYS:HE2	1:l:56:GLU:HG3	1.81	0.60
1:K:101:LEU:HD22	1:K:120:LEU:HD13	1.84	0.60
1:k:106:VAL:HG13	3:k:381:HOH:O	2.02	0.60
1:f:1:MET:HB2	1:w:95:TYR:OH	2.01	0.60
1:N:24:GLN:NE2	3:N:319:HOH:O	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:53:ARG:NH1	3:Q:295:HOH:O	2.35	0.59
1:W:117:ALA:O	1:W:121:GLU:HG3	2.02	0.59
1:S:107:MET:HE3	1:S:107:MET:O	2.01	0.59
1:f:24:GLN:NE2	1:f:78:ARG:H	2.00	0.59
1:u:98:LEU:O	1:u:102:LYS:HG3	2.02	0.59
1:F:152:GLN:O	1:V:156:ARG:HG2	2.02	0.59
1:H:139:GLU:O	1:H:143:LYS:HG3	2.03	0.59
1:b:62:ILE:HG13	3:b:252:HOH:O	2.02	0.59
1:C:52:MET:SD	2:C:200:HEM:ND	2.75	0.59
1:E:157:PRO:HD3	1:W:39:GLU:HB3	1.84	0.59
1:w:28:HIS:CD2	1:w:86:GLN:HG2	2.37	0.59
1:C:18:GLU:OE2	1:C:51:GLU:OE2	2.20	0.59
1:E:74:ILE:HG12	1:E:75:GLY:N	2.11	0.59
1:L:39:GLU:C	3:L:399:HOH:O	2.45	0.59
1:M:77:LEU:HD12	1:M:77:LEU:N	2.18	0.59
2:F:200:HEM:HHC	2:F:200:HEM:HBB2	1.84	0.59
1:G:6:ASP:OD1	1:G:9:ARG:NH2	2.34	0.59
1:X:1:MET:C	3:X:343:HOH:O	2.44	0.59
1:a:50:ASP:OD1	1:a:53:ARG:NH2	2.35	0.59
1:k:1:MET:HE3	1:k:64:LEU:HD21	1.84	0.59
1:l:28:HIS:CD2	1:l:86:GLN:HG2	2.38	0.59
3:l:243:HOH:O	1:p:159:THR:HG22	2.03	0.59
1:m:18:GLU:OE2	1:m:51:GLU:OE2	2.20	0.59
1:q:25:TYR:OH	1:q:94:GLU:OE1	2.21	0.59
1:U:18:GLU:OE2	1:U:51:GLU:OE2	2.21	0.59
1:U:32:GLN:HG3	1:U:86:GLN:HE22	1.68	0.59
1:e:56:GLU:HG3	1:f:30:LYS:HE2	1.84	0.59
1:m:101:LEU:HD22	1:m:120:LEU:HD22	1.84	0.59
1:M:23:ASN:OD1	2:M:200:HEM:CBB	2.50	0.59
1:w:94:GLU:OE2	1:w:127:GLU:OE1	2.20	0.59
2:C:200:HEM:HMA1	2:C:200:HEM:CBA	2.33	0.59
1:A:94:GLU:OE2	1:A:134:LEU:HD11	2.03	0.59
1:D:151:ALA:O	1:D:154:VAL:HG22	2.03	0.59
1:G:28:HIS:O	1:G:32:GLN:HG3	2.03	0.59
1:e:156:ARG:CD	3:e:318:HOH:O	2.48	0.59
1:l:45:ARG:HG2	1:l:49:PHE:HE1	1.68	0.59
2:o:200:HEM:CMD	3:p:212:HOH:O	2.50	0.59
1:t:14:GLN:NE2	1:t:18:GLU:OE1	2.33	0.59
1:t:74:ILE:HG12	1:t:75:GLY:N	2.18	0.59
1:F:84:ARG:HH11	1:F:84:ARG:HG3	1.68	0.58
1:n:118:VAL:O	1:n:122:LYS:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:149:TYR:C	1:o:149:TYR:CD2	2.81	0.58
1:t:78:ARG:NE	3:t:367:HOH:O	2.35	0.58
1:T:24:GLN:NE2	1:T:78:ARG:H	2.01	0.58
1:f:2:GLN:CG	3:f:277:HOH:O	2.41	0.58
1:V:91:LEU:CD2	1:V:131:ILE:HG23	2.34	0.58
1:t:9:ARG:CG	1:t:9:ARG:NH1	2.62	0.58
1:x:49:PHE:CD2	2:x:200:HEM:HBD2	2.37	0.58
2:P:200:HEM:HHC	2:P:200:HEM:CBB	2.28	0.58
1:k:26:PHE:CE1	2:k:200:HEM:HBC2	2.38	0.58
1:t:100:ARG:HG2	1:t:101:LEU:HD23	1.85	0.58
1:q:74:ILE:HD11	1:q:77:LEU:HD13	1.85	0.58
1:s:78:ARG:NH1	1:s:92:ALA:CB	2.65	0.58
1:L:18:GLU:HA	1:L:18:GLU:OE1	2.03	0.58
1:R:135:GLU:O	1:R:139:GLU:HG3	2.04	0.58
1:c:78:ARG:NH1	1:c:92:ALA:HB1	2.19	0.58
1:i:79:ILE:HG12	3:i:305:HOH:O	2.03	0.58
1:w:52:MET:HE3	3:w:265:HOH:O	2.03	0.58
1:H:49:PHE:HA	1:H:52:MET:HG3	1.86	0.58
1:K:18:GLU:O	1:K:22:ILE:HG13	2.03	0.58
1:O:45:ARG:NH2	3:O:229:HOH:O	2.36	0.58
1:b:158:PRO:HB2	1:v:137:GLN:HE22	1.66	0.58
2:g:200:HEM:HBA2	2:g:200:HEM:CMA	2.34	0.58
1:l:107:MET:O	1:l:111:LYS:HG2	2.04	0.58
1:n:22:ILE:HD11	1:n:52:MET:HA	1.85	0.58
1:D:131:ILE:O	1:D:135:GLU:HG3	2.03	0.58
1:G:16:THR:HG21	3:G:272:HOH:O	2.04	0.58
1:G:102:LYS:HB2	1:G:103:PRO:HD2	1.84	0.58
1:L:18:GLU:OE1	1:L:51:GLU:OE1	2.21	0.58
1:S:94:GLU:OE2	1:S:127:GLU:HB3	2.02	0.58
1:h:53:ARG:NE	3:h:249:HOH:O	2.35	0.58
1:m:101:LEU:CD2	1:m:120:LEU:HD22	2.34	0.58
1:v:74:ILE:HG12	1:v:75:GLY:H	1.68	0.58
1:Q:40:LEU:HB2	1:Q:153:CYS:HB3	1.86	0.58
1:f:32:GLN:NE2	3:f:272:HOH:O	2.37	0.58
1:h:112:GLN:HG3	3:h:232:HOH:O	2.04	0.58
1:k:26:PHE:CE2	2:k:200:HEM:CBC	2.85	0.58
1:M:85:GLU:HG3	3:M:353:HOH:O	2.02	0.57
1:S:64:LEU:HD23	1:S:64:LEU:C	2.29	0.57
1:h:53:ARG:NH1	3:h:251:HOH:O	2.37	0.57
1:t:152:GLN:HE22	1:x:156:ARG:NH2	2.01	0.57
1:D:90:ASP:O	1:D:93:ILE:HG22	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:4:ASP:OD2	1:W:4:ASP:C	2.47	0.57
1:l:94:GLU:OE1	1:l:127:GLU:OE1	2.22	0.57
1:K:159:THR:CG2	3:K:261:HOH:O	2.52	0.57
1:c:50:ASP:OD1	1:c:53:ARG:NH2	2.37	0.57
1:h:38:THR:CG2	1:h:159:THR:HG23	2.33	0.57
1:A:123:ILE:O	1:A:127:GLU:HG2	2.04	0.57
1:H:40:LEU:HD13	3:H:388:HOH:O	2.03	0.57
1:K:159:THR:HG23	3:K:261:HOH:O	2.05	0.57
1:s:84:ARG:HD3	3:s:258:HOH:O	2.03	0.57
1:u:97:VAL:HG11	1:u:127:GLU:HG3	1.86	0.57
3:O:272:HOH:O	2:P:200:HEM:HBA1	2.05	0.57
1:P:9:ARG:NH1	3:P:353:HOH:O	2.37	0.57
1:U:9:ARG:CG	3:U:450:HOH:O	2.42	0.57
1:k:74:ILE:HD11	1:k:77:LEU:HD13	1.85	0.57
1:v:18:GLU:OE2	1:v:51:GLU:OE2	2.21	0.57
1:E:74:ILE:HG12	1:E:75:GLY:O	2.05	0.57
1:I:94:GLU:OE2	1:I:127:GLU:CD	2.48	0.57
1:a:39:GLU:HB3	1:s:157:PRO:HD3	1.86	0.57
1:S:50:ASP:OD1	1:S:53:ARG:NH2	2.38	0.57
1:K:113:ASP:HB2	3:K:239:HOH:O	2.03	0.57
1:M:93:ILE:HD12	3:M:355:HOH:O	2.04	0.57
1:i:78:ARG:N	3:i:281:HOH:O	2.37	0.57
1:B:74:ILE:HG22	3:B:391:HOH:O	2.04	0.57
1:a:22:ILE:HD11	1:a:52:MET:HA	1.87	0.57
1:l:102:LYS:CB	1:l:103:PRO:CD	2.82	0.57
1:E:102:LYS:CB	1:E:103:PRO:CD	2.82	0.57
1:M:94:GLU:OE2	1:M:127:GLU:OE1	2.23	0.57
1:d:102:LYS:HE2	1:m:112:GLN:O	2.05	0.57
2:k:200:HEM:HBB2	2:k:200:HEM:CHC	2.22	0.57
1:v:94:GLU:OE1	1:v:134:LEU:HD12	2.05	0.57
1:f:123:ILE:O	1:f:127:GLU:HG2	2.04	0.56
2:P:200:HEM:HBB2	2:P:200:HEM:CHC	2.21	0.56
1:T:118:VAL:CG1	1:T:122:LYS:HE3	2.34	0.56
1:d:77:LEU:CD1	1:d:77:LEU:N	2.67	0.56
1:o:56:GLU:HG2	1:p:30:LYS:HE2	1.87	0.56
1:A:27:LEU:HD23	1:A:79:ILE:HD12	1.86	0.56
1:B:50:ASP:OD2	1:B:53:ARG:NH2	2.39	0.56
1:G:98:LEU:O	1:G:102:LYS:HG3	2.06	0.56
1:d:152:GLN:HE22	1:o:156:ARG:NH2	1.94	0.56
1:v:159:THR:HA	3:v:324:HOH:O	2.06	0.56
1:I:22:ILE:HD11	1:I:52:MET:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:56:GLU:HG3	1:N:30:LYS:HE2	1.87	0.56
1:X:78:ARG:HD3	3:X:347:HOH:O	2.04	0.56
1:c:52:MET:HE2	2:c:200:HEM:NC	2.20	0.56
1:x:12:ASN:HD21	1:x:70:ASN:H	1.51	0.56
1:D:110:GLU:CG	3:D:202:HOH:O	2.54	0.56
1:e:113:ASP:CG	1:e:116:SER:HB2	2.31	0.56
1:r:73:ARG:N	3:r:287:HOH:O	2.31	0.56
1:v:97:VAL:HG12	1:v:101:LEU:HD12	1.86	0.56
1:C:109:ARG:HB2	3:C:364:HOH:O	2.05	0.56
2:L:200:HEM:HBB2	2:L:200:HEM:CHC	2.18	0.56
1:R:52:MET:CE	2:R:200:HEM:C4C	2.89	0.56
2:j:200:HEM:HBB2	2:j:200:HEM:CHC	2.09	0.56
1:o:84:ARG:CB	1:o:141:MET:HE1	2.35	0.56
1:p:50:ASP:OD2	1:p:53:ARG:NH2	2.38	0.56
1:B:90:ASP:O	1:B:93:ILE:HG22	2.06	0.56
1:T:74:ILE:HG12	1:T:75:GLY:N	2.21	0.56
1:a:27:LEU:HD23	1:a:79:ILE:HD12	1.87	0.56
1:e:147:GLU:CD	1:e:147:GLU:H	2.13	0.56
1:j:25:TYR:N	1:j:25:TYR:CD1	2.74	0.56
1:O:1:MET:HE3	1:O:64:LEU:HD21	1.88	0.56
1:a:149:TYR:C	1:a:149:TYR:CD2	2.83	0.56
1:l:1:MET:HE3	1:l:64:LEU:HD23	1.88	0.56
1:n:131:ILE:O	1:n:135:GLU:HG3	2.06	0.56
1:q:123:ILE:O	1:q:127:GLU:HG2	2.05	0.56
1:r:123:ILE:O	1:r:127:GLU:HG2	2.05	0.56
1:x:119:LEU:HD12	1:x:119:LEU:O	2.05	0.56
1:O:64:LEU:C	1:O:64:LEU:HD23	2.30	0.56
1:R:82:THR:O	1:R:86:GLN:HG3	2.05	0.56
1:c:61:ARG:NH2	1:c:115:THR:HB	2.21	0.56
1:c:64:LEU:HD23	1:c:64:LEU:C	2.31	0.56
1:e:123:ILE:O	1:e:127:GLU:HG2	2.06	0.56
1:k:155:SER:HB2	3:k:313:HOH:O	2.06	0.56
1:l:45:ARG:HG2	1:l:49:PHE:CE1	2.41	0.56
1:o:53:ARG:NH2	3:o:327:HOH:O	2.33	0.56
1:F:123:ILE:O	1:F:127:GLU:HG2	2.05	0.56
1:K:21:ALA:HB2	1:K:93:ILE:CD1	2.36	0.56
1:Q:21:ALA:HB2	1:Q:93:ILE:HD13	1.87	0.56
1:c:94:GLU:OE2	1:c:127:GLU:OE2	2.24	0.56
1:E:148:LEU:HA	1:W:148:LEU:HD21	1.88	0.55
1:I:18:GLU:OE1	1:I:51:GLU:OE1	2.24	0.55
1:I:149:TYR:C	1:I:149:TYR:CD2	2.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:18:GLU:OE2	1:V:51:GLU:OE2	2.24	0.55
1:d:64:LEU:HD23	1:d:64:LEU:C	2.31	0.55
1:e:97:VAL:HG13	1:e:101:LEU:CD1	2.36	0.55
1:H:33:ASP:OD1	1:H:38:THR:HG22	2.06	0.55
1:M:101:LEU:HD22	1:M:120:LEU:HD13	1.88	0.55
1:Q:100:ARG:CB	1:Q:100:ARG:CZ	2.84	0.55
1:d:50:ASP:OD1	1:d:53:ARG:NH2	2.40	0.55
1:j:33:ASP:OD1	1:j:38:THR:HG22	2.04	0.55
1:s:93:ILE:O	1:s:97:VAL:HG23	2.06	0.55
1:Q:100:ARG:HB2	1:Q:100:ARG:CZ	2.36	0.55
1:a:18:GLU:O	1:a:22:ILE:HG13	2.06	0.55
1:h:53:ARG:NH2	3:h:249:HOH:O	2.36	0.55
1:A:102:LYS:HB2	1:A:103:PRO:CD	2.35	0.55
1:G:102:LYS:HB2	1:G:103:PRO:HD3	1.88	0.55
1:Q:21:ALA:HB2	1:Q:93:ILE:CD1	2.35	0.55
1:G:84:ARG:NH2	3:G:271:HOH:O	2.25	0.55
1:Q:134:LEU:HD21	3:Q:224:HOH:O	2.06	0.55
1:W:12:ASN:CG	3:W:257:HOH:O	2.49	0.55
1:x:49:PHE:CE2	2:x:200:HEM:C1A	2.95	0.55
1:B:12:ASN:HD21	1:B:70:ASN:H	1.52	0.55
1:L:28:HIS:NE2	1:L:86:GLN:HG2	2.22	0.55
1:i:77:LEU:CB	3:i:281:HOH:O	2.54	0.55
1:l:102:LYS:CB	1:l:103:PRO:HD2	2.36	0.55
1:B:52:MET:HE1	2:B:200:HEM:C4C	2.42	0.55
1:R:149:TYR:C	1:R:149:TYR:CD2	2.84	0.55
1:c:1:MET:CA	3:r:260:HOH:O	2.43	0.55
1:i:121:GLU:HG2	1:k:114:THR:HG21	1.87	0.55
1:s:52:MET:HG2	2:t:200:HEM:NB	2.22	0.55
1:B:51:GLU:CD	1:B:54:HIS:ND1	2.65	0.55
1:K:21:ALA:HB2	1:K:93:ILE:HD13	1.89	0.55
1:P:19:LEU:HA	1:P:22:ILE:HD12	1.87	0.55
1:q:4:ASP:OD2	1:q:6:ASP:HB2	2.07	0.55
1:G:112:GLN:O	1:P:102:LYS:HE3	2.07	0.55
1:J:14:GLN:O	1:J:18:GLU:HG2	2.07	0.55
1:K:18:GLU:OE1	1:K:51:GLU:OE1	2.24	0.55
1:d:123:ILE:O	1:d:127:GLU:HG2	2.07	0.55
1:C:129:GLU:HG3	3:C:312:HOH:O	2.06	0.55
1:F:149:TYR:C	1:F:149:TYR:CD2	2.84	0.55
1:I:151:ALA:HA	3:I:398:HOH:O	2.06	0.55
1:x:27:LEU:HD23	1:x:79:ILE:CD1	2.32	0.55
1:E:28:HIS:NE2	1:E:86:GLN:HG2	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:15:LEU:O	1:U:15:LEU:HD12	2.07	0.54
1:n:123:ILE:O	1:n:127:GLU:HG2	2.06	0.54
1:o:40:LEU:HB2	1:o:153:CYS:HB3	1.90	0.54
1:B:52:MET:CE	2:B:200:HEM:NC	2.70	0.54
1:d:49:PHE:HB3	1:d:53:ARG:HH12	1.71	0.54
1:r:84:ARG:NH1	1:r:84:ARG:HG3	2.22	0.54
1:D:14:GLN:O	1:D:18:GLU:HG2	2.07	0.54
1:G:25:TYR:OH	1:G:94:GLU:OE2	2.24	0.54
1:H:52:MET:HB3	2:H:200:HEM:CHB	2.38	0.54
1:P:52:MET:HB3	2:P:200:HEM:CHD	2.37	0.54
1:W:1:MET:HE3	1:W:64:LEU:HD23	1.85	0.54
1:X:97:VAL:HG11	1:X:127:GLU:HG3	1.89	0.54
1:k:102:LYS:NZ	3:k:316:HOH:O	2.38	0.54
1:t:17:SER:HB2	1:t:100:ARG:NH2	2.22	0.54
1:K:73:ARG:HB3	3:K:282:HOH:O	2.06	0.54
1:O:1:MET:HE3	1:O:64:LEU:CD2	2.37	0.54
1:O:1:MET:N	3:O:219:HOH:O	2.29	0.54
1:o:18:GLU:OE1	1:o:51:GLU:OE1	2.25	0.54
1:w:48:SER:CB	3:w:265:HOH:O	2.36	0.54
1:E:101:LEU:HD22	1:E:120:LEU:HD22	1.89	0.54
1:k:1:MET:HE3	1:k:64:LEU:HD23	1.88	0.54
1:m:153:CYS:SG	3:m:216:HOH:O	2.24	0.54
1:U:52:MET:HB3	2:U:200:HEM:CHB	2.38	0.54
1:e:43:HIS:CE1	1:e:47:GLU:OE2	2.61	0.54
1:g:22:ILE:HD11	1:g:52:MET:HA	1.88	0.54
1:r:84:ARG:NH2	3:r:293:HOH:O	2.36	0.54
1:t:25:TYR:OH	1:t:94:GLU:OE1	2.26	0.54
1:t:156:ARG:HH12	1:x:152:GLN:HE21	1.54	0.54
1:I:1:MET:HE3	1:I:64:LEU:HD21	1.89	0.54
1:J:61:ARG:NH2	1:J:115:THR:HB	2.23	0.54
1:Q:94:GLU:OE1	1:Q:127:GLU:CG	2.50	0.54
1:u:87:PHE:HE2	1:u:141:MET:HE3	1.73	0.54
1:v:49:PHE:CE2	2:v:200:HEM:HBA2	2.42	0.54
2:C:200:HEM:ND	1:D:52:MET:SD	2.81	0.54
1:G:91:LEU:HD21	1:G:135:GLU:HG3	1.90	0.54
1:e:157:PRO:HD3	1:w:39:GLU:HB3	1.89	0.54
1:m:91:LEU:HD22	1:m:95:TYR:CE2	2.43	0.54
1:F:64:LEU:C	1:F:64:LEU:HD23	2.32	0.54
1:K:91:LEU:HD11	1:K:135:GLU:CG	2.38	0.54
1:M:102:LYS:CB	1:M:103:PRO:CD	2.86	0.54
2:e:200:HEM:HBC2	2:e:200:HEM:CMC	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:64:LEU:O	1:h:64:LEU:HD23	2.07	0.54
1:i:132:ASP:HA	3:i:277:HOH:O	2.07	0.54
1:n:19:LEU:HD22	2:n:200:HEM:CBB	2.38	0.54
1:o:17:SER:CB	1:o:100:ARG:NH2	2.71	0.54
1:q:14:GLN:O	1:q:18:GLU:HG2	2.07	0.54
1:s:78:ARG:HH12	1:s:92:ALA:HB1	1.70	0.54
1:c:18:GLU:OE1	1:c:18:GLU:HA	2.08	0.54
1:F:19:LEU:HD22	2:F:200:HEM:HBB1	1.89	0.53
1:J:82:THR:O	1:J:86:GLN:HG3	2.08	0.53
1:P:131:ILE:O	1:P:135:GLU:HG3	2.07	0.53
1:S:98:LEU:HD13	3:S:343:HOH:O	2.08	0.53
1:V:4:ASP:OD1	1:V:111:LYS:HD2	2.06	0.53
1:X:78:ARG:HH11	1:X:92:ALA:HB1	1.69	0.53
1:e:97:VAL:HG13	1:e:101:LEU:HD12	1.90	0.53
1:I:93:ILE:CD1	3:I:384:HOH:O	2.57	0.53
1:M:149:TYR:C	1:M:149:TYR:CD2	2.86	0.53
1:P:87:PHE:HE2	1:P:141:MET:HE3	1.72	0.53
1:Q:22:ILE:HD11	1:Q:52:MET:HA	1.89	0.53
2:g:200:HEM:HHD	2:g:200:HEM:CBC	2.33	0.53
1:i:50:ASP:OD2	1:i:53:ARG:NH2	2.36	0.53
1:o:17:SER:HB2	1:o:100:ARG:NH2	2.23	0.53
1:B:102:LYS:HE2	1:D:112:GLN:O	2.07	0.53
1:C:70:ASN:ND2	1:C:73:ARG:H	2.06	0.53
1:D:149:TYR:C	1:D:149:TYR:CD2	2.86	0.53
1:L:39:GLU:CB	3:L:399:HOH:O	2.37	0.53
1:V:94:GLU:OE1	1:V:127:GLU:CB	2.51	0.53
1:t:141:MET:HE3	1:t:146:GLU:CD	2.33	0.53
2:C:200:HEM:HBC1	1:D:71:TYR:HE1	1.73	0.53
1:V:4:ASP:CG	1:V:111:LYS:HD2	2.34	0.53
1:g:139:GLU:O	1:g:143:LYS:HG3	2.09	0.53
1:u:78:ARG:NH1	3:u:309:HOH:O	2.42	0.53
1:S:107:MET:CE	1:S:107:MET:O	2.57	0.53
1:O:60:ASP:OD1	1:P:30:LYS:CE	2.56	0.53
1:V:110:GLU:HG3	3:V:267:HOH:O	2.09	0.53
1:m:10:LEU:HD21	1:m:104:GLY:HA3	1.91	0.53
1:p:97:VAL:HG22	1:p:100:ARG:HH21	1.74	0.53
1:t:91:LEU:HD21	1:t:135:GLU:HG2	1.91	0.53
1:t:141:MET:CE	1:t:146:GLU:CD	2.82	0.53
1:K:31:MET:HE1	1:K:80:GLY:O	2.09	0.53
1:T:61:ARG:NH2	1:T:115:THR:HB	2.24	0.53
1:d:89:ALA:O	1:d:92:ALA:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:123:ILE:O	1:j:127:GLU:HG2	2.09	0.53
1:q:64:LEU:C	1:q:64:LEU:HD23	2.33	0.53
1:u:117:ALA:O	1:u:121:GLU:HG3	2.09	0.53
1:D:39:GLU:HB3	1:N:157:PRO:HD3	1.89	0.53
1:H:149:TYR:C	1:H:149:TYR:CD2	2.87	0.53
1:K:91:LEU:HD11	1:K:135:GLU:HG3	1.90	0.53
1:W:84:ARG:HD3	3:W:270:HOH:O	2.09	0.53
1:j:22:ILE:HD11	1:j:52:MET:HA	1.91	0.53
1:j:149:TYR:C	1:j:149:TYR:CD2	2.87	0.53
1:t:141:MET:HE2	1:t:146:GLU:OE1	2.09	0.53
1:u:123:ILE:O	1:u:127:GLU:HG2	2.09	0.53
1:w:149:TYR:CD2	1:w:149:TYR:O	2.62	0.53
1:O:87:PHE:CE2	1:O:141:MET:HE3	2.37	0.53
1:B:9:ARG:NH2	1:f:74:ILE:O	2.41	0.53
1:N:28:HIS:CD2	1:N:86:GLN:HG2	2.44	0.53
1:O:1:MET:CE	1:O:64:LEU:HD21	2.39	0.53
1:k:93:ILE:HD13	3:k:390:HOH:O	2.07	0.53
1:t:27:LEU:HD23	1:t:79:ILE:HD12	1.90	0.53
1:t:141:MET:HE3	1:t:146:GLU:HG3	1.90	0.53
1:x:101:LEU:HD22	1:x:120:LEU:HD22	1.91	0.53
1:C:39:GLU:O	1:F:157:PRO:HG3	2.08	0.52
1:E:28:HIS:CD2	1:E:86:GLN:HG2	2.44	0.52
1:E:156:ARG:HD3	3:W:216:HOH:O	2.07	0.52
1:T:13:GLU:OE1	1:T:100:ARG:HD3	2.09	0.52
1:D:66:ASP:HB2	3:D:251:HOH:O	2.09	0.52
1:b:82:THR:O	1:b:86:GLN:HG3	2.09	0.52
1:o:39:GLU:HB3	1:r:157:PRO:HD3	1.90	0.52
1:r:21:ALA:O	1:r:22:ILE:C	2.50	0.52
1:B:9:ARG:NH1	1:f:76:SER:OG	2.36	0.52
1:D:110:GLU:HG2	3:D:202:HOH:O	2.08	0.52
1:I:102:LYS:HE3	3:I:415:HOH:O	2.08	0.52
1:Q:56:GLU:HG3	1:R:30:LYS:HE2	1.91	0.52
1:b:102:LYS:HB2	1:b:103:PRO:CD	2.39	0.52
1:q:113:ASP:CG	1:q:116:SER:HB2	2.34	0.52
1:K:157:PRO:HG3	1:Q:39:GLU:O	2.09	0.52
1:N:29:SER:HB3	1:N:44:THR:HB	1.91	0.52
1:O:102:LYS:N	1:O:103:PRO:HD2	2.25	0.52
1:W:14:GLN:NE2	1:W:18:GLU:OE1	2.42	0.52
1:C:61:ARG:NH2	1:C:115:THR:HB	2.24	0.52
2:C:200:HEM:HHD	2:C:200:HEM:HBC2	1.91	0.52
1:e:78:ARG:NH2	1:e:92:ALA:HB3	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:87:PHE:HD2	1:k:141:MET:HE3	1.74	0.52
1:l:119:LEU:HD12	1:l:119:LEU:C	2.34	0.52
1:r:84:ARG:HG3	1:r:84:ARG:HH11	1.74	0.52
1:D:93:ILE:CB	3:D:245:HOH:O	2.53	0.52
1:D:94:GLU:OE2	1:D:127:GLU:OE2	2.28	0.52
1:R:52:MET:HE1	2:R:200:HEM:CHD	2.40	0.52
2:c:200:HEM:HBB2	2:c:200:HEM:CHC	2.34	0.52
1:g:38:THR:HG21	1:g:159:THR:HG23	1.91	0.52
2:g:200:HEM:CBC	1:h:26:PHE:CE2	2.93	0.52
1:s:159:THR:HG21	3:s:201:HOH:O	2.06	0.52
2:P:200:HEM:HHA	2:P:200:HEM:HBA2	1.92	0.52
1:W:18:GLU:HG3	1:W:58:ILE:CD1	2.39	0.52
1:q:9:ARG:HG2	1:q:13:GLU:OE1	2.10	0.52
2:q:200:HEM:HBB2	2:q:200:HEM:HMB2	1.91	0.52
1:B:52:MET:CE	2:B:200:HEM:C4C	2.92	0.52
1:R:18:GLU:OE2	1:R:51:GLU:OE2	2.26	0.52
2:e:200:HEM:CGD	3:e:367:HOH:O	2.57	0.52
1:m:87:PHE:CE2	1:m:141:MET:HE3	2.44	0.52
1:v:131:ILE:O	1:v:135:GLU:HG3	2.09	0.52
1:E:29:SER:HB3	1:E:44:THR:HG22	1.92	0.52
1:Q:18:GLU:OE1	1:Q:51:GLU:OE2	2.27	0.52
1:d:18:GLU:OE2	1:d:51:GLU:OE2	2.27	0.52
1:k:93:ILE:O	1:k:96:ASP:HB2	2.09	0.52
1:I:93:ILE:CB	3:I:384:HOH:O	2.48	0.52
1:J:18:GLU:OE1	1:J:51:GLU:OE2	2.27	0.52
1:Q:112:GLN:HA	3:Q:210:HOH:O	2.10	0.52
2:a:200:HEM:NC	1:b:52:MET:HG2	2.25	0.52
1:h:157:PRO:HG3	1:p:39:GLU:O	2.09	0.52
1:F:84:ARG:HG3	1:F:84:ARG:NH1	2.24	0.51
1:Q:147:GLU:CD	1:Q:147:GLU:H	2.18	0.51
1:R:61:ARG:NH2	1:R:115:THR:HB	2.25	0.51
1:g:1:MET:HA	3:g:356:HOH:O	2.08	0.51
1:i:30:LYS:HE2	1:j:56:GLU:HG3	1.92	0.51
1:p:53:ARG:CG	3:p:212:HOH:O	2.48	0.51
1:w:15:LEU:HB2	1:w:58:ILE:HG21	1.91	0.51
1:w:133:TYR:O	1:w:137:GLN:HG2	2.09	0.51
1:x:93:ILE:O	1:x:93:ILE:HG13	2.10	0.51
1:E:78:ARG:HB2	1:E:89:ALA:HB1	1.92	0.51
1:F:18:GLU:OE1	1:F:51:GLU:OE1	2.29	0.51
1:Q:9:ARG:HH11	1:Q:9:ARG:HB3	1.74	0.51
1:U:149:TYR:C	1:U:149:TYR:CD2	2.87	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:24:GLN:NE2	1:W:78:ARG:H	2.09	0.51
1:s:18:GLU:OE2	1:s:54:HIS:CB	2.58	0.51
2:C:200:HEM:HHC	2:C:200:HEM:HBB2	1.92	0.51
1:E:107:MET:O	1:E:111:LYS:HG2	2.10	0.51
1:n:74:ILE:HG23	1:n:74:ILE:O	2.10	0.51
1:q:53:ARG:HG2	3:q:365:HOH:O	2.10	0.51
1:i:2:GLN:HG3	3:i:223:HOH:O	2.10	0.51
1:x:149:TYR:C	1:x:149:TYR:CD2	2.89	0.51
1:D:27:LEU:HD23	1:D:79:ILE:HD12	1.92	0.51
1:N:95:TYR:HD1	3:N:317:HOH:O	1.93	0.51
1:b:4:ASP:CB	1:b:7:VAL:HG23	2.39	0.51
1:F:131:ILE:O	1:F:135:GLU:HG3	2.10	0.51
1:G:117:ALA:O	1:G:121:GLU:HG3	2.11	0.51
1:S:25:TYR:OH	1:S:94:GLU:OE1	2.27	0.51
1:h:18:GLU:OE2	1:h:51:GLU:OE2	2.27	0.51
1:c:43:HIS:O	1:c:47:GLU:HG2	2.10	0.51
1:d:62:ILE:CG2	1:d:69:PRO:HG3	2.40	0.51
1:e:4:ASP:CG	1:e:5:PRO:HD2	2.36	0.51
1:e:90:ASP:O	1:e:93:ILE:HG22	2.10	0.51
1:k:64:LEU:HD23	1:k:64:LEU:C	2.36	0.51
1:E:147:GLU:OE1	1:E:147:GLU:N	2.37	0.51
1:j:52:MET:HE2	2:j:200:HEM:NB	2.26	0.51
1:o:39:GLU:O	1:r:157:PRO:HG3	2.10	0.51
1:K:51:GLU:OE2	1:K:51:GLU:HA	2.10	0.51
1:P:123:ILE:O	1:P:127:GLU:HG2	2.11	0.51
1:U:24:GLN:NE2	1:U:78:ARG:H	2.08	0.51
1:e:107:MET:O	1:e:111:LYS:HG2	2.11	0.51
1:h:13:GLU:OE2	1:h:100:ARG:HD3	2.11	0.51
1:o:133:TYR:O	1:o:137:GLN:HG2	2.10	0.51
1:q:9:ARG:O	1:q:13:GLU:HG3	2.11	0.51
1:I:33:ASP:OD1	1:I:38:THR:HG22	2.11	0.51
1:M:94:GLU:OE1	1:M:130:HIS:ND1	2.36	0.51
1:k:1:MET:CE	1:k:64:LEU:CD2	2.87	0.51
1:n:149:TYR:CD2	1:n:149:TYR:C	2.88	0.51
1:T:123:ILE:O	1:T:127:GLU:HG2	2.11	0.50
1:V:159:THR:CG2	3:V:250:HOH:O	2.31	0.50
1:C:26:PHE:O	1:C:30:LYS:HG2	2.10	0.50
1:E:94:GLU:OE1	1:E:127:GLU:OE2	2.29	0.50
1:G:105:ILE:HD13	1:G:121:GLU:HG2	1.94	0.50
1:i:141:MET:HG2	1:i:146:GLU:HG3	1.93	0.50
1:e:78:ARG:NH2	1:e:92:ALA:CB	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:27:LEU:HD23	1:o:79:ILE:HD12	1.92	0.50
1:q:156:ARG:NH2	1:w:152:GLN:OE1	2.42	0.50
1:f:18:GLU:OE2	1:f:51:GLU:OE1	2.29	0.50
1:E:10:LEU:CD2	3:E:259:HOH:O	2.60	0.50
1:F:133:TYR:O	1:F:137:GLN:HG2	2.12	0.50
1:J:78:ARG:HB2	1:J:89:ALA:HB1	1.92	0.50
1:W:90:ASP:O	1:W:94:GLU:HG2	2.12	0.50
2:X:200:HEM:HBC2	2:X:200:HEM:CMC	2.42	0.50
1:h:91:LEU:HD11	1:h:135:GLU:HG3	1.93	0.50
1:o:53:ARG:CZ	3:o:327:HOH:O	2.59	0.50
1:p:22:ILE:HD11	1:p:52:MET:HA	1.93	0.50
1:r:143:LYS:CE	3:r:265:HOH:O	2.59	0.50
1:v:49:PHE:HE2	2:v:200:HEM:HBA2	1.76	0.50
1:B:77:LEU:HD23	1:B:79:ILE:HD11	1.93	0.50
1:C:78:ARG:NH2	3:C:363:HOH:O	2.43	0.50
2:C:200:HEM:HHC	2:C:200:HEM:CBB	2.42	0.50
1:G:112:GLN:HB3	1:P:102:LYS:HB3	1.94	0.50
1:T:94:GLU:OE2	1:T:130:HIS:CE1	2.64	0.50
1:h:64:LEU:HD23	1:h:64:LEU:C	2.36	0.50
1:h:94:GLU:OE2	1:h:127:GLU:OE1	2.29	0.50
1:l:1:MET:HE3	1:l:64:LEU:CD2	2.41	0.50
1:q:64:LEU:HD23	1:q:64:LEU:O	2.11	0.50
1:C:139:GLU:O	1:C:143:LYS:HG3	2.11	0.50
1:M:9:ARG:HG3	1:M:9:ARG:NH1	2.26	0.50
1:T:25:TYR:OH	1:T:94:GLU:OE2	2.27	0.50
1:W:22:ILE:HD11	1:W:52:MET:HA	1.92	0.50
1:i:156:ARG:NH2	1:p:152:GLN:HE22	1.95	0.50
1:t:39:GLU:O	1:u:157:PRO:HG3	2.12	0.50
1:B:139:GLU:CD	3:B:363:HOH:O	2.55	0.50
1:D:25:TYR:OH	1:D:94:GLU:OE1	2.20	0.50
1:P:97:VAL:HG11	1:P:127:GLU:HG3	1.92	0.50
1:e:157:PRO:HD3	1:w:39:GLU:CB	2.42	0.50
1:w:28:HIS:NE2	1:w:86:GLN:HG2	2.26	0.50
1:A:94:GLU:OE2	1:A:134:LEU:HD12	2.11	0.50
1:E:102:LYS:CB	3:R:401:HOH:O	2.60	0.50
1:K:53:ARG:HG3	3:L:373:HOH:O	2.10	0.50
1:e:101:LEU:HD22	1:e:120:LEU:HD22	1.93	0.50
1:U:26:PHE:CD2	2:U:200:HEM:HAC	2.46	0.49
1:w:74:ILE:HG22	3:w:251:HOH:O	2.12	0.49
1:M:159:THR:HG21	3:M:357:HOH:O	2.12	0.49
1:h:39:GLU:OE2	1:h:155:SER:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:84:ARG:HD3	3:n:330:HOH:O	2.12	0.49
1:q:18:GLU:OE1	1:q:51:GLU:OE1	2.30	0.49
1:X:16:THR:HG23	3:X:403:HOH:O	2.12	0.49
1:J:113:ASP:OD2	1:J:116:SER:OG	2.29	0.49
1:K:149:TYR:C	1:K:149:TYR:CD2	2.90	0.49
1:a:33:ASP:OD1	1:a:38:THR:HG22	2.12	0.49
1:e:52:MET:HB3	2:e:200:HEM:CHD	2.42	0.49
1:q:22:ILE:HG13	1:q:51:GLU:HB3	1.94	0.49
1:A:80:GLY:HA3	1:A:86:GLN:HG3	1.95	0.49
1:K:33:ASP:OD1	1:K:38:THR:HG22	2.13	0.49
1:i:2:GLN:CG	3:i:223:HOH:O	2.60	0.49
1:w:25:TYR:OH	1:w:94:GLU:OE1	2.29	0.49
1:A:113:ASP:C	1:A:113:ASP:OD1	2.54	0.49
2:I:200:HEM:CHB	1:J:52:MET:HB3	2.43	0.49
1:J:23:ASN:ND2	3:J:317:HOH:O	2.41	0.49
1:W:45:ARG:NH1	3:W:263:HOH:O	2.35	0.49
1:h:97:VAL:HG11	1:h:127:GLU:HG3	1.95	0.49
1:i:31:MET:HE1	1:i:80:GLY:O	2.12	0.49
1:r:53:ARG:O	1:r:57:GLU:HG3	2.13	0.49
1:u:101:LEU:HD22	1:u:120:LEU:HD22	1.93	0.49
1:w:13:GLU:OE2	1:w:100:ARG:HD3	2.12	0.49
1:A:39:GLU:OE1	3:A:330:HOH:O	2.20	0.49
1:X:120:LEU:O	1:X:124:VAL:HG23	2.13	0.49
1:b:102:LYS:HE3	3:d:242:HOH:O	2.13	0.49
1:r:4:ASP:HB3	1:r:7:VAL:CG2	2.43	0.49
1:x:123:ILE:O	1:x:127:GLU:HG2	2.13	0.49
1:J:91:LEU:HD21	1:J:135:GLU:HG3	1.95	0.49
1:L:98:LEU:O	1:L:102:LYS:HG3	2.12	0.49
1:N:22:ILE:HD11	1:N:52:MET:HA	1.95	0.49
1:R:49:PHE:CZ	2:R:200:HEM:C3D	3.01	0.49
1:e:17:SER:HA	3:e:387:HOH:O	2.12	0.49
1:m:123:ILE:O	1:m:127:GLU:HG2	2.13	0.49
1:p:91:LEU:O	1:p:95:TYR:HB2	2.12	0.49
1:H:123:ILE:O	1:H:127:GLU:HG2	2.12	0.49
1:M:52:MET:HG2	2:M:200:HEM:C4C	2.47	0.49
1:q:94:GLU:OE2	1:q:127:GLU:OE1	2.31	0.49
1:t:74:ILE:CG1	1:t:75:GLY:N	2.76	0.49
1:I:148:LEU:HD21	1:L:148:LEU:HA	1.95	0.48
1:L:1:MET:HA	3:L:327:HOH:O	2.12	0.48
1:O:147:GLU:CD	1:O:147:GLU:H	2.20	0.48
2:S:200:HEM:HBB1	1:T:19:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:84:ARG:NE	3:V:306:HOH:O	2.42	0.48
1:p:18:GLU:OE2	1:p:51:GLU:OE2	2.30	0.48
1:q:98:LEU:O	1:q:102:LYS:HG3	2.13	0.48
1:r:18:GLU:O	1:r:22:ILE:HG13	2.13	0.48
1:s:1:MET:N	3:s:250:HOH:O	2.24	0.48
1:C:14:GLN:HA	1:C:14:GLN:OE1	2.12	0.48
1:D:20:THR:N	3:D:287:HOH:O	2.45	0.48
1:J:91:LEU:HD11	1:J:135:GLU:HG2	1.95	0.48
1:U:82:THR:O	1:U:86:GLN:HG3	2.13	0.48
1:W:31:MET:HE1	1:W:80:GLY:O	2.13	0.48
1:d:22:ILE:HD11	1:d:52:MET:HA	1.95	0.48
1:f:90:ASP:O	1:f:93:ILE:HG22	2.13	0.48
1:p:87:PHE:CE2	1:p:141:MET:HE3	2.48	0.48
1:w:26:PHE:CE2	1:w:30:LYS:HD3	2.48	0.48
1:P:53:ARG:NH1	2:P:200:HEM:O1D	2.47	0.48
1:T:84:ARG:HD3	3:T:219:HOH:O	2.12	0.48
1:b:102:LYS:CB	1:b:103:PRO:CD	2.91	0.48
1:k:151:ALA:O	1:k:154:VAL:HG22	2.13	0.48
1:o:50:ASP:OD1	1:o:53:ARG:NH2	2.46	0.48
1:t:24:GLN:HE21	1:t:78:ARG:H	1.55	0.48
1:w:13:GLU:HG3	3:w:258:HOH:O	2.13	0.48
1:M:52:MET:HG2	2:M:200:HEM:NC	2.28	0.48
1:M:91:LEU:HD21	1:M:135:GLU:HG3	1.94	0.48
1:S:62:ILE:HG22	1:S:69:PRO:HD3	1.95	0.48
1:U:34:ASN:HB2	3:U:326:HOH:O	2.13	0.48
1:U:97:VAL:HG22	1:U:100:ARG:HH21	1.77	0.48
1:W:77:LEU:HB2	1:X:72:GLN:OE1	2.13	0.48
1:g:84:ARG:NH2	1:g:146:GLU:OE2	2.44	0.48
1:m:49:PHE:HE2	2:n:200:HEM:HAA1	1.78	0.48
1:v:4:ASP:OD1	1:v:6:ASP:HB2	2.14	0.48
1:M:109:ARG:NH1	3:M:358:HOH:O	2.31	0.48
1:S:49:PHE:CZ	2:S:200:HEM:C2A	3.02	0.48
2:j:200:HEM:HH2	2:j:200:HEM:HBC2	1.94	0.48
2:q:200:HEM:HBB1	1:r:19:LEU:CD2	2.43	0.48
1:M:23:ASN:OD1	2:M:200:HEM:HBB1	2.11	0.48
1:N:149:TYR:CE1	1:O:158:PRO:HG2	2.48	0.48
1:O:22:ILE:HD11	1:O:52:MET:HA	1.96	0.48
1:Q:114:THR:O	1:Q:118:VAL:HG23	2.13	0.48
1:X:159:THR:HG21	3:X:399:HOH:O	2.13	0.48
1:f:28:HIS:C	3:f:272:HOH:O	2.55	0.48
1:n:28:HIS:CD2	1:n:86:GLN:HG2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:200:HEM:HBB2	2:q:200:HEM:CMB	2.43	0.48
1:G:124:VAL:O	1:G:128:GLU:HG3	2.14	0.48
1:H:53:ARG:NH2	3:H:383:HOH:O	2.35	0.48
1:K:2:GLN:NE2	1:K:66:ASP:OD2	2.47	0.48
1:d:149:TYR:CE1	1:n:158:PRO:HG2	2.49	0.48
1:k:87:PHE:CE2	1:k:141:MET:HE3	2.48	0.48
2:o:200:HEM:CBA	3:o:321:HOH:O	2.29	0.48
1:F:82:THR:OG1	1:F:85:GLU:HG3	2.13	0.48
1:K:30:LYS:HE2	1:L:56:GLU:HG3	1.96	0.48
1:M:102:LYS:CB	1:M:103:PRO:HD3	2.44	0.48
2:P:200:HEM:HBA2	2:P:200:HEM:CHA	2.43	0.48
1:S:151:ALA:O	1:S:154:VAL:HG22	2.13	0.48
1:U:4:ASP:HB3	1:U:7:VAL:HG21	1.92	0.48
1:i:77:LEU:HB3	3:i:281:HOH:O	2.13	0.48
2:o:200:HEM:HBB1	1:p:23:ASN:OD1	2.14	0.48
1:r:27:LEU:HD23	1:r:79:ILE:HD12	1.96	0.48
1:w:107:MET:O	1:w:111:LYS:HG2	2.14	0.48
1:B:151:ALA:O	1:B:154:VAL:HG22	2.13	0.48
1:G:53:ARG:NH1	2:H:200:HEM:O1D	2.44	0.48
1:d:77:LEU:N	1:d:77:LEU:HD12	2.28	0.48
1:m:17:SER:OG	1:m:100:ARG:NH2	2.47	0.48
1:p:113:ASP:OD2	1:p:116:SER:OG	2.27	0.48
1:t:27:LEU:HD23	1:t:79:ILE:CD1	2.44	0.48
1:M:94:GLU:CD	1:M:130:HIS:HD1	2.20	0.48
1:U:8:LEU:HD21	1:U:65:LEU:HB2	1.95	0.48
1:f:90:ASP:O	1:f:93:ILE:CG2	2.61	0.48
1:f:148:LEU:O	1:f:151:ALA:HB3	2.14	0.48
1:k:10:LEU:HD21	1:k:104:GLY:CA	2.44	0.48
1:l:102:LYS:HB2	1:l:103:PRO:CD	2.41	0.48
1:t:113:ASP:CG	1:t:116:SER:HB2	2.38	0.48
1:w:2:GLN:NE2	1:w:66:ASP:OD2	2.47	0.48
2:C:200:HEM:CMB	1:D:26:PHE:CZ	2.98	0.47
1:O:30:LYS:HE2	1:P:60:ASP:OD1	2.13	0.47
1:Q:123:ILE:O	1:Q:127:GLU:OE1	2.32	0.47
1:V:33:ASP:OD1	1:V:38:THR:HG22	2.14	0.47
1:W:33:ASP:OD1	1:W:38:THR:HG22	2.14	0.47
2:e:200:HEM:HBB2	2:e:200:HEM:CHC	2.18	0.47
1:h:127:GLU:CD	3:h:257:HOH:O	2.56	0.47
1:p:90:ASP:O	1:p:93:ILE:HG23	2.13	0.47
1:w:130:HIS:CE1	3:w:288:HOH:O	2.66	0.47
1:H:144:LEU:HD11	3:I:398:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:52:MET:HB3	2:L:200:HEM:CHD	2.44	0.47
1:Q:158:PRO:O	1:Q:159:THR:C	2.56	0.47
1:d:18:GLU:O	1:d:22:ILE:HG13	2.15	0.47
1:g:61:ARG:NH2	1:g:115:THR:HB	2.29	0.47
1:t:111:LYS:HE3	3:t:342:HOH:O	2.14	0.47
1:E:142:ASP:OD2	3:E:281:HOH:O	2.20	0.47
1:I:1:MET:HE3	1:I:64:LEU:CD2	2.45	0.47
1:M:102:LYS:HB2	1:M:103:PRO:HD3	1.97	0.47
1:j:78:ARG:HB2	1:j:89:ALA:HB1	1.96	0.47
1:n:113:ASP:OD2	1:n:116:SER:OG	2.23	0.47
1:p:147:GLU:HB2	3:p:260:HOH:O	2.12	0.47
1:D:9:ARG:HD3	3:D:286:HOH:O	2.13	0.47
2:a:200:HEM:HBB2	2:a:200:HEM:CHC	2.24	0.47
1:n:18:GLU:OE1	1:n:51:GLU:OE1	2.31	0.47
1:q:122:LYS:HD2	3:q:388:HOH:O	2.14	0.47
1:F:101:LEU:HA	1:F:101:LEU:HD23	1.58	0.47
1:K:133:TYR:O	1:K:137:GLN:HG2	2.14	0.47
1:V:88:GLU:OE2	3:V:315:HOH:O	2.20	0.47
1:f:6:ASP:OD1	1:f:9:ARG:NH2	2.42	0.47
1:h:33:ASP:OD1	1:h:38:THR:HG22	2.14	0.47
2:o:200:HEM:CBB	1:p:23:ASN:OD1	2.62	0.47
1:E:102:LYS:CG	3:R:401:HOH:O	2.48	0.47
1:G:49:PHE:HE2	2:H:200:HEM:HAA1	1.80	0.47
1:H:94:GLU:OE1	1:H:127:GLU:OE1	2.33	0.47
1:M:14:GLN:NE2	1:M:18:GLU:OE2	2.48	0.47
1:P:61:ARG:NH1	1:P:115:THR:HG21	2.29	0.47
1:Q:1:MET:HB3	3:Q:228:HOH:O	2.14	0.47
3:T:325:HOH:O	1:V:1:MET:HE3	2.11	0.47
2:a:200:HEM:HBC2	2:a:200:HEM:HMC1	1.96	0.47
1:A:1:MET:CE	1:A:64:LEU:CD2	2.92	0.47
1:H:82:THR:O	1:H:86:GLN:HG3	2.14	0.47
1:I:61:ARG:NH2	1:I:115:THR:HB	2.29	0.47
1:I:137:GLN:OE1	1:L:158:PRO:HB2	2.15	0.47
1:J:4:ASP:CB	3:J:220:HOH:O	2.52	0.47
1:J:87:PHE:CE2	1:J:141:MET:HE3	2.48	0.47
1:L:18:GLU:O	1:L:22:ILE:HG13	2.15	0.47
1:M:77:LEU:N	1:M:77:LEU:CD1	2.77	0.47
1:Q:9:ARG:HH11	1:Q:9:ARG:CB	2.28	0.47
1:V:149:TYR:C	1:V:149:TYR:CD2	2.93	0.47
1:f:31:MET:HE1	1:f:80:GLY:O	2.14	0.47
1:k:18:GLU:OE1	1:k:51:GLU:OE1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:106:VAL:O	1:t:110:GLU:HG3	2.15	0.47
1:v:152:GLN:OE1	1:v:152:GLN:HA	2.15	0.47
1:E:10:LEU:HD21	3:E:259:HOH:O	2.14	0.47
1:K:94:GLU:OE1	1:K:127:GLU:CD	2.58	0.47
1:R:108:CYS:HB3	1:R:117:ALA:HB2	1.97	0.47
1:S:1:MET:HE3	1:S:64:LEU:CD2	2.44	0.47
1:W:18:GLU:HG3	1:W:58:ILE:HD12	1.96	0.47
1:g:87:PHE:HE2	1:g:141:MET:HE3	1.80	0.47
1:w:36:GLY:HA2	1:w:159:THR:OG1	2.15	0.47
1:F:6:ASP:OD1	1:F:9:ARG:NH1	2.39	0.47
2:L:200:HEM:HBD2	2:L:200:HEM:HHA	1.97	0.47
1:d:157:PRO:HD3	1:r:39:GLU:HB3	1.96	0.47
1:l:106:VAL:O	1:l:110:GLU:HG3	2.15	0.47
1:t:82:THR:O	1:t:86:GLN:HG3	2.14	0.47
1:u:139:GLU:O	1:u:143:LYS:HG3	2.15	0.47
1:Q:133:TYR:O	1:Q:137:GLN:HG2	2.15	0.47
1:X:123:ILE:O	1:X:127:GLU:HG2	2.15	0.47
1:c:53:ARG:NH1	2:c:200:HEM:O1A	2.46	0.47
1:e:47:GLU:O	1:e:51:GLU:HG2	2.15	0.47
1:q:52:MET:CE	2:q:200:HEM:NB	2.78	0.47
1:x:87:PHE:HE2	1:x:141:MET:HE3	1.80	0.47
1:A:22:ILE:HG12	1:A:52:MET:HG3	1.95	0.46
1:B:158:PRO:O	1:B:159:THR:C	2.58	0.46
1:C:39:GLU:C	1:F:157:PRO:HG3	2.40	0.46
1:C:52:MET:HG2	2:C:200:HEM:NB	2.30	0.46
1:H:107:MET:C	1:H:107:MET:SD	2.98	0.46
1:R:98:LEU:O	1:R:102:LYS:HG3	2.14	0.46
1:c:78:ARG:NH2	3:c:376:HOH:O	2.47	0.46
1:N:102:LYS:N	1:N:103:PRO:HD2	2.29	0.46
1:V:84:ARG:HD2	3:V:306:HOH:O	2.15	0.46
1:e:52:MET:HB3	2:e:200:HEM:C1D	2.50	0.46
1:m:102:LYS:N	1:m:103:PRO:HD2	2.30	0.46
1:n:65:LEU:HA	1:n:65:LEU:HD23	1.51	0.46
1:o:97:VAL:HG11	1:o:127:GLU:HG3	1.96	0.46
1:p:27:LEU:O	1:p:31:MET:HG3	2.15	0.46
1:q:4:ASP:CG	1:q:5:PRO:HD2	2.41	0.46
1:q:19:LEU:HB3	3:q:374:HOH:O	2.15	0.46
1:t:52:MET:HG2	2:t:200:HEM:NC	2.30	0.46
1:t:70:ASN:C	1:t:70:ASN:HD22	2.23	0.46
1:C:86:GLN:HB3	3:C:380:HOH:O	2.12	0.46
1:E:98:LEU:HD11	1:E:131:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:17:SER:HB2	1:H:100:ARG:NH2	2.30	0.46
1:L:10:LEU:HD21	1:L:104:GLY:HA3	1.97	0.46
1:U:113:ASP:CG	1:U:116:SER:HB2	2.40	0.46
1:k:19:LEU:HA	1:k:22:ILE:HD12	1.97	0.46
1:q:152:GLN:OE1	1:w:156:ARG:NH2	2.43	0.46
1:C:49:PHE:CZ	2:C:200:HEM:HAD1	2.50	0.46
1:O:144:LEU:HB3	1:O:148:LEU:HD23	1.96	0.46
1:U:51:GLU:OE2	1:U:51:GLU:HA	2.15	0.46
1:t:102:LYS:N	1:t:103:PRO:HD2	2.30	0.46
1:P:28:HIS:CD2	1:P:86:GLN:HG2	2.51	0.46
1:R:37:PHE:HE1	1:R:150:SER:HB3	1.80	0.46
1:C:40:LEU:HB2	1:C:153:CYS:HB3	1.98	0.46
2:L:200:HEM:HBC2	2:L:200:HEM:CHD	2.41	0.46
1:N:123:ILE:O	1:N:127:GLU:HG2	2.15	0.46
1:p:87:PHE:HE2	1:p:141:MET:HE3	1.81	0.46
1:p:133:TYR:O	1:p:137:GLN:HG2	2.14	0.46
1:q:52:MET:HG2	2:q:200:HEM:C1C	2.50	0.46
1:x:61:ARG:HD3	3:x:397:HOH:O	2.15	0.46
1:A:18:GLU:OE2	1:A:51:GLU:OE2	2.32	0.46
1:E:25:TYR:CG	3:E:207:HOH:O	2.69	0.46
1:P:142:ASP:CG	3:P:406:HOH:O	2.58	0.46
1:X:61:ARG:NH1	3:X:397:HOH:O	2.29	0.46
1:g:78:ARG:NH1	1:g:92:ALA:HB1	2.31	0.46
1:o:25:TYR:OH	1:o:94:GLU:OE1	2.26	0.46
1:p:17:SER:OG	1:p:100:ARG:NH2	2.48	0.46
1:E:93:ILE:O	1:E:93:ILE:HG13	2.12	0.46
1:G:47:GLU:OE1	1:G:47:GLU:HA	2.16	0.46
1:H:53:ARG:NE	3:H:383:HOH:O	2.45	0.46
1:R:112:GLN:HB3	3:R:401:HOH:O	2.16	0.46
1:S:135:GLU:O	1:S:139:GLU:HG3	2.16	0.46
1:a:156:ARG:NH2	1:g:152:GLN:OE1	2.47	0.46
1:i:81:GLN:HA	1:i:81:GLN:OE1	2.16	0.46
1:m:1:MET:HE3	1:m:64:LEU:CD2	2.46	0.46
1:o:53:ARG:NH1	2:o:200:HEM:O1A	2.49	0.46
1:o:78:ARG:NH1	1:o:92:ALA:HB1	2.30	0.46
1:x:48:SER:O	1:x:52:MET:HG3	2.16	0.46
1:C:1:MET:HB2	1:R:95:TYR:OH	2.15	0.46
1:G:146:GLU:OE1	3:G:243:HOH:O	2.20	0.46
1:P:1:MET:CE	1:P:64:LEU:HD21	2.46	0.46
1:l:74:ILE:HG12	1:l:75:GLY:N	2.30	0.46
2:C:200:HEM:ND	2:C:200:HEM:NA	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1:MET:HB3	1:J:1:MET:HE2	1.29	0.46
1:e:51:GLU:OE2	1:e:51:GLU:HA	2.16	0.46
1:g:27:LEU:HD23	1:g:79:ILE:HD12	1.98	0.46
1:o:64:LEU:C	1:o:64:LEU:HD23	2.41	0.46
1:w:43:HIS:CE1	1:w:133:TYR:CE2	3.03	0.46
1:O:2:GLN:HG2	1:O:66:ASP:HB3	1.98	0.45
1:P:148:LEU:O	1:P:151:ALA:HB3	2.16	0.45
1:f:1:MET:HE2	1:w:131:ILE:HG22	1.97	0.45
2:g:200:HEM:CBC	1:h:26:PHE:CZ	3.00	0.45
1:k:47:GLU:HG3	1:k:130:HIS:NE2	2.32	0.45
1:w:91:LEU:HD21	1:w:135:GLU:HG3	1.98	0.45
2:C:200:HEM:HBC1	1:D:71:TYR:CE1	2.50	0.45
1:F:87:PHE:HE2	1:F:141:MET:HE3	1.81	0.45
1:F:91:LEU:HA	1:F:91:LEU:HD23	1.68	0.45
1:M:51:GLU:OE2	3:M:360:HOH:O	2.21	0.45
1:Q:66:ASP:OD2	3:Q:305:HOH:O	2.21	0.45
1:T:94:GLU:OE1	1:T:134:LEU:HD12	2.16	0.45
1:V:142:ASP:CG	3:V:314:HOH:O	2.58	0.45
1:h:122:LYS:NZ	3:h:245:HOH:O	2.48	0.45
1:w:111:LYS:HD2	3:w:283:HOH:O	2.15	0.45
1:C:113:ASP:CG	1:C:116:SER:HB2	2.42	0.45
2:C:200:HEM:HBC2	2:C:200:HEM:CHD	2.46	0.45
1:J:63:LEU:HD23	1:J:63:LEU:HA	1.81	0.45
1:L:4:ASP:HA	1:L:5:PRO:HD3	1.81	0.45
1:L:17:SER:HB2	1:L:100:ARG:HH22	1.81	0.45
1:S:18:GLU:OE2	1:S:51:GLU:OE2	2.33	0.45
1:T:133:TYR:O	1:T:137:GLN:HG2	2.16	0.45
1:U:32:GLN:HE21	1:U:86:GLN:HE21	1.62	0.45
1:b:64:LEU:HD23	1:b:64:LEU:C	2.42	0.45
1:c:1:MET:HB2	1:r:95:TYR:OH	2.16	0.45
1:e:157:PRO:HG3	1:w:40:LEU:HA	1.98	0.45
1:n:135:GLU:O	1:n:139:GLU:HG3	2.15	0.45
1:s:91:LEU:HD11	1:s:135:GLU:HG2	1.99	0.45
1:G:149:TYR:C	1:G:149:TYR:CD2	2.94	0.45
1:H:156:ARG:NH2	3:H:409:HOH:O	2.48	0.45
1:S:117:ALA:O	1:S:121:GLU:HG3	2.16	0.45
1:b:96:ASP:OD1	3:b:236:HOH:O	2.21	0.45
2:c:200:HEM:HHC	2:c:200:HEM:CBB	2.40	0.45
1:d:156:ARG:HA	1:d:157:PRO:HA	1.73	0.45
2:e:200:HEM:HBC2	2:e:200:HEM:HMC1	1.98	0.45
1:h:129:GLU:HB2	3:h:238:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:94:GLU:HA	1:o:94:GLU:OE2	2.17	0.45
1:r:120:LEU:O	1:r:124:VAL:HG23	2.16	0.45
1:D:18:GLU:OE2	1:D:51:GLU:OE1	2.35	0.45
1:a:84:ARG:HD3	3:a:319:HOH:O	2.16	0.45
1:a:132:ASP:OD1	3:a:350:HOH:O	2.21	0.45
1:i:77:LEU:CA	3:i:281:HOH:O	2.64	0.45
1:o:84:ARG:O	1:o:88:GLU:HG2	2.17	0.45
1:o:96:ASP:HB2	3:o:370:HOH:O	2.15	0.45
1:C:4:ASP:HA	1:C:5:PRO:HD3	1.80	0.45
1:H:91:LEU:HD21	1:H:135:GLU:HG3	1.98	0.45
1:J:147:GLU:CD	1:J:147:GLU:N	2.74	0.45
1:N:148:LEU:HD21	1:O:148:LEU:HA	1.99	0.45
1:O:93:ILE:O	1:O:97:VAL:HG23	2.16	0.45
1:S:78:ARG:NH1	1:S:92:ALA:HB1	2.31	0.45
1:d:10:LEU:HD21	1:d:104:GLY:HA3	1.99	0.45
1:m:87:PHE:HE2	1:m:141:MET:HE3	1.81	0.45
1:r:84:ARG:HH11	1:r:84:ARG:CG	2.28	0.45
1:u:135:GLU:O	1:u:139:GLU:HG3	2.16	0.45
2:x:200:HEM:HHC	2:x:200:HEM:HBB2	1.99	0.45
1:I:66:ASP:CG	1:I:66:ASP:O	2.58	0.45
1:L:97:VAL:HG11	1:L:127:GLU:HG3	1.99	0.45
1:L:100:ARG:NH1	3:L:388:HOH:O	2.46	0.45
1:L:149:TYR:CE1	1:P:158:PRO:HG2	2.51	0.45
1:O:53:ARG:HD2	3:O:212:HOH:O	2.16	0.45
1:R:2:GLN:NE2	3:R:351:HOH:O	2.45	0.45
1:V:110:GLU:OE1	3:V:248:HOH:O	2.20	0.45
1:V:135:GLU:O	1:V:139:GLU:HG3	2.17	0.45
1:g:61:ARG:NH1	1:g:64:LEU:HD22	2.32	0.45
1:p:2:GLN:HG2	3:p:251:HOH:O	2.14	0.45
1:C:30:LYS:HE2	1:D:56:GLU:HG3	1.97	0.45
1:D:28:HIS:O	1:D:32:GLN:HG3	2.17	0.45
1:I:32:GLN:HG3	1:I:86:GLN:HE22	1.80	0.45
1:O:102:LYS:N	1:O:103:PRO:CD	2.80	0.45
1:R:1:MET:N	3:R:362:HOH:O	2.27	0.45
1:V:78:ARG:HD2	3:V:308:HOH:O	2.17	0.45
1:h:13:GLU:CD	1:h:100:ARG:HD3	2.42	0.45
1:h:69:PRO:CD	3:h:260:HOH:O	2.40	0.45
1:p:30:LYS:HA	1:p:30:LYS:HD2	1.89	0.45
1:q:1:MET:CE	1:q:64:LEU:HD21	2.39	0.45
1:q:24:GLN:HE22	1:q:78:ARG:H	1.62	0.45
1:q:62:ILE:CG2	1:q:69:PRO:HD3	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:38:THR:HG21	1:G:159:THR:CG2	2.44	0.45
1:L:36:GLY:O	1:L:154:VAL:HG12	2.17	0.45
2:P:200:HEM:HBC2	2:P:200:HEM:CMC	2.46	0.45
1:A:102:LYS:CB	1:A:103:PRO:CD	2.94	0.45
1:C:32:GLN:NE2	3:C:380:HOH:O	2.50	0.45
1:C:109:ARG:HD2	3:C:364:HOH:O	2.17	0.45
1:G:120:LEU:O	1:G:124:VAL:HG23	2.17	0.45
1:J:102:LYS:N	1:J:103:PRO:HD2	2.32	0.45
2:R:200:HEM:HHC	2:R:200:HEM:CBB	2.47	0.45
1:S:64:LEU:HD23	1:S:64:LEU:O	2.16	0.45
1:U:91:LEU:HD11	1:U:135:GLU:HG2	1.99	0.45
1:X:78:ARG:HH12	1:X:92:ALA:HB1	1.69	0.45
1:e:87:PHE:CE2	1:e:141:MET:CE	2.95	0.45
1:n:83:LEU:HD23	1:n:83:LEU:HA	1.77	0.45
1:q:18:GLU:OE1	1:q:51:GLU:CD	2.60	0.45
1:s:18:GLU:OE2	1:s:54:HIS:HB2	2.17	0.45
1:C:144:LEU:HB3	1:C:148:LEU:HD23	1.99	0.44
1:D:78:ARG:NH1	1:D:92:ALA:HB1	2.32	0.44
1:K:93:ILE:O	1:K:97:VAL:HG23	2.17	0.44
1:Q:50:ASP:OD1	1:Q:53:ARG:NH2	2.49	0.44
1:d:158:PRO:HB2	1:r:137:GLN:OE1	2.17	0.44
1:r:53:ARG:NH1	3:r:264:HOH:O	2.37	0.44
1:H:52:MET:HE1	2:H:200:HEM:C4C	2.53	0.44
1:L:94:GLU:OE1	1:L:127:GLU:HB3	2.17	0.44
1:P:18:GLU:OE2	1:P:51:GLU:OE2	2.34	0.44
1:Q:33:ASP:OD1	1:Q:38:THR:HG22	2.18	0.44
1:Q:38:THR:CG2	1:Q:159:THR:CG2	2.89	0.44
1:Q:39:GLU:OE2	1:Q:155:SER:HB3	2.17	0.44
1:W:94:GLU:OE2	1:W:94:GLU:HA	2.18	0.44
1:a:18:GLU:OE2	1:a:51:GLU:OE2	2.35	0.44
1:i:64:LEU:HD23	1:i:64:LEU:C	2.42	0.44
1:s:107:MET:O	1:s:111:LYS:HG2	2.18	0.44
1:w:94:GLU:CD	1:w:127:GLU:OE1	2.60	0.44
1:x:61:ARG:NH2	1:x:115:THR:HB	2.32	0.44
1:O:97:VAL:HG12	1:O:101:LEU:HD12	1.99	0.44
1:Q:30:LYS:HE2	1:R:60:ASP:OD1	2.17	0.44
1:e:73:ARG:HD2	1:e:74:ILE:H	1.82	0.44
1:g:2:GLN:CG	3:g:354:HOH:O	2.65	0.44
1:g:38:THR:CG2	1:g:159:THR:HG23	2.48	0.44
1:q:74:ILE:HD11	1:q:77:LEU:CD1	2.48	0.44
1:r:94:GLU:OE1	1:r:130:HIS:ND1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:s:2:GLN:CD	3:s:257:HOH:O	2.61	0.44
1:t:52:MET:HG2	2:t:200:HEM:C4C	2.52	0.44
1:v:4:ASP:HB3	1:v:7:VAL:HG23	2.00	0.44
1:G:61:ARG:HA	1:G:61:ARG:HD2	1.86	0.44
1:R:90:ASP:O	1:R:93:ILE:HG22	2.18	0.44
1:r:15:LEU:HD12	1:r:15:LEU:O	2.17	0.44
1:B:51:GLU:HG3	1:B:54:HIS:HB2	1.99	0.44
1:E:98:LEU:HD11	1:E:131:ILE:CD1	2.48	0.44
1:H:80:GLY:HA3	1:H:86:GLN:HG2	2.00	0.44
1:P:7:VAL:HA	1:P:107:MET:HE1	1.98	0.44
1:a:93:ILE:O	1:a:97:VAL:HG23	2.18	0.44
2:I:200:HEM:HHA	2:I:200:HEM:HBA2	1.99	0.44
1:K:73:ARG:O	3:K:282:HOH:O	2.21	0.44
1:M:102:LYS:HB2	1:M:103:PRO:CD	2.47	0.44
1:O:20:THR:HG23	1:O:77:LEU:HD12	2.00	0.44
1:O:94:GLU:OE1	1:O:127:GLU:OE1	2.35	0.44
1:P:7:VAL:O	1:P:10:LEU:HB3	2.17	0.44
1:d:39:GLU:HB3	1:n:157:PRO:HD3	1.99	0.44
1:g:4:ASP:HA	1:g:5:PRO:HD3	1.83	0.44
1:r:4:ASP:HB3	1:r:7:VAL:HG23	1.99	0.44
1:w:68:LEU:HB3	3:w:275:HOH:O	2.17	0.44
1:A:74:ILE:O	1:e:9:ARG:NH2	2.51	0.44
1:E:94:GLU:CD	1:E:127:GLU:OE2	2.61	0.44
1:F:28:HIS:CE1	1:F:86:GLN:HA	2.53	0.44
1:G:33:ASP:OD1	1:G:38:THR:HG22	2.18	0.44
1:H:93:ILE:O	1:H:93:ILE:HG13	2.18	0.44
1:J:22:ILE:HD11	1:J:52:MET:HA	2.00	0.44
1:Q:30:LYS:CE	1:R:60:ASP:OD1	2.66	0.44
2:X:200:HEM:HHA	3:X:304:HOH:O	2.18	0.44
1:b:87:PHE:CE2	1:b:141:MET:HE3	2.53	0.44
1:f:94:GLU:OE2	1:f:127:GLU:OE1	2.36	0.44
1:i:49:PHE:CZ	2:j:200:HEM:C3D	3.05	0.44
1:j:30:LYS:HA	1:j:30:LYS:HD2	1.70	0.44
1:k:30:LYS:HE2	1:l:56:GLU:CG	2.47	0.44
1:v:135:GLU:O	1:v:139:GLU:HG3	2.17	0.44
1:H:9:ARG:NE	3:H:435:HOH:O	2.51	0.44
1:L:52:MET:HE2	2:L:200:HEM:C4B	2.53	0.44
1:M:17:SER:CB	1:M:100:ARG:NH2	2.81	0.44
1:X:33:ASP:O	3:X:378:HOH:O	2.21	0.44
1:X:34:ASN:ND2	3:X:404:HOH:O	2.22	0.44
1:a:54:HIS:O	1:a:58:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:22:ILE:HD11	1:f:52:MET:HA	1.99	0.44
1:n:43:HIS:HE1	1:n:47:GLU:OE2	2.00	0.44
1:p:82:THR:O	1:p:86:GLN:HG3	2.17	0.44
1:q:93:ILE:O	1:q:97:VAL:HG23	2.18	0.44
1:s:52:MET:CE	2:t:200:HEM:NC	2.76	0.44
1:E:71:TYR:CD2	1:F:27:LEU:HD22	2.52	0.44
1:I:22:ILE:CD1	1:I:52:MET:HA	2.48	0.44
1:L:50:ASP:HB3	3:L:321:HOH:O	2.18	0.44
1:f:61:ARG:NH2	1:f:115:THR:HB	2.33	0.44
1:i:14:GLN:O	1:i:18:GLU:HG2	2.18	0.44
1:j:53:ARG:NH2	3:j:346:HOH:O	2.20	0.44
1:l:123:ILE:O	1:l:127:GLU:HG2	2.17	0.44
1:q:107:MET:SD	1:q:107:MET:C	3.00	0.44
1:u:143:LYS:HE3	3:u:255:HOH:O	2.18	0.44
1:C:97:VAL:HG11	1:C:127:GLU:HG3	2.00	0.43
1:R:37:PHE:CE1	1:R:150:SER:HB3	2.53	0.43
1:l:28:HIS:CG	1:l:86:GLN:HG2	2.53	0.43
1:m:49:PHE:CZ	2:n:200:HEM:C2A	3.06	0.43
1:E:18:GLU:OE1	1:E:51:GLU:OE2	2.35	0.43
1:E:102:LYS:HA	3:R:401:HOH:O	2.17	0.43
1:M:52:MET:HE2	2:M:200:HEM:C4B	2.54	0.43
1:X:134:LEU:HA	1:X:134:LEU:HD23	1.75	0.43
1:k:28:HIS:CD2	1:k:86:GLN:HG2	2.52	0.43
1:q:140:LEU:HD23	1:q:140:LEU:HA	1.89	0.43
1:r:151:ALA:O	1:r:154:VAL:HG22	2.18	0.43
1:H:159:THR:HG22	3:H:360:HOH:O	2.18	0.43
1:I:101:LEU:HD22	1:I:120:LEU:HD22	2.00	0.43
1:O:37:PHE:CD2	1:O:83:LEU:HD21	2.53	0.43
1:X:33:ASP:CG	3:X:378:HOH:O	2.61	0.43
1:d:18:GLU:OE2	1:d:18:GLU:HA	2.19	0.43
1:e:43:HIS:O	1:e:47:GLU:HG2	2.17	0.43
3:h:261:HOH:O	1:i:35:TRP:HA	2.18	0.43
1:p:87:PHE:HB2	1:p:138:LEU:HD21	2.00	0.43
1:A:74:ILE:O	1:A:74:ILE:HG23	2.19	0.43
1:W:72:GLN:O	1:W:72:GLN:HG3	2.18	0.43
1:t:39:GLU:C	1:u:157:PRO:HG3	2.43	0.43
1:M:11:LEU:HD23	1:M:11:LEU:HA	1.77	0.43
1:Q:74:ILE:O	1:Q:74:ILE:CG2	2.64	0.43
1:S:39:GLU:OE2	1:S:155:SER:HB3	2.19	0.43
1:W:149:TYR:CD2	1:W:149:TYR:C	2.96	0.43
1:c:133:TYR:O	1:c:137:GLN:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:31:MET:HE2	1:e:86:GLN:NE2	2.33	0.43
1:e:137:GLN:HA	3:e:375:HOH:O	2.18	0.43
1:i:18:GLU:OE2	1:i:51:GLU:OE2	2.35	0.43
1:i:51:GLU:HA	1:i:51:GLU:OE2	2.19	0.43
1:x:87:PHE:CE2	1:x:141:MET:HE3	2.53	0.43
1:A:18:GLU:OE2	1:A:18:GLU:HA	2.19	0.43
1:A:22:ILE:HD13	1:A:52:MET:HG2	2.00	0.43
1:A:102:LYS:HB2	1:A:103:PRO:HD2	2.00	0.43
1:G:43:HIS:O	1:G:46:ALA:HB3	2.18	0.43
1:M:102:LYS:N	1:M:103:PRO:HD2	2.34	0.43
1:Q:38:THR:HG21	1:Q:159:THR:CG2	2.46	0.43
1:Q:158:PRO:HA	3:Q:272:HOH:O	2.18	0.43
1:T:131:ILE:HG22	1:V:1:MET:HE2	2.00	0.43
1:X:18:GLU:HA	1:X:18:GLU:OE2	2.19	0.43
1:X:149:TYR:CD2	1:X:149:TYR:C	2.95	0.43
1:b:18:GLU:HA	1:b:18:GLU:OE2	2.19	0.43
1:k:159:THR:HG23	3:k:301:HOH:O	2.19	0.43
1:l:21:ALA:HB2	1:l:93:ILE:HD13	2.00	0.43
1:l:149:TYR:CD2	1:l:149:TYR:C	2.96	0.43
1:t:141:MET:HE3	1:t:146:GLU:CG	2.48	0.43
1:u:9:ARG:HA	3:u:240:HOH:O	2.17	0.43
1:v:49:PHE:N	1:v:49:PHE:CD1	2.87	0.43
1:C:6:ASP:OD2	3:C:368:HOH:O	2.21	0.43
1:C:80:GLY:HA3	1:C:86:GLN:HG3	2.01	0.43
1:D:90:ASP:O	1:D:93:ILE:CG2	2.65	0.43
1:H:4:ASP:HB3	1:H:7:VAL:CG2	2.48	0.43
1:Q:13:GLU:OE2	1:Q:100:ARG:HD3	2.18	0.43
1:b:25:TYR:OH	1:b:94:GLU:OE2	2.35	0.43
1:b:43:HIS:CE1	1:b:133:TYR:CZ	3.06	0.43
1:h:102:LYS:HB2	1:h:103:PRO:CD	2.48	0.43
1:l:138:LEU:HD23	1:l:138:LEU:HA	1.75	0.43
1:o:56:GLU:CG	1:p:26:PHE:HZ	2.18	0.43
1:G:9:ARG:HG3	3:G:304:HOH:O	2.17	0.43
1:M:28:HIS:O	1:M:32:GLN:HG3	2.19	0.43
1:Q:130:HIS:CE1	1:Q:134:LEU:HD11	2.54	0.43
1:r:25:TYR:OH	1:r:94:GLU:OE2	2.36	0.43
1:x:55:ALA:HB3	2:x:200:HEM:HBC2	2.01	0.43
1:E:131:ILE:O	1:E:135:GLU:HG3	2.18	0.43
1:I:134:LEU:HD23	1:I:134:LEU:HA	1.67	0.43
1:M:158:PRO:O	1:M:159:THR:C	2.61	0.43
1:M:159:THR:CG2	3:M:357:HOH:O	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:4:ASP:CB	1:U:7:VAL:HG23	2.44	0.43
1:U:131:ILE:O	1:U:135:GLU:HG3	2.19	0.43
1:a:4:ASP:OD2	1:a:6:ASP:HB2	2.18	0.43
1:f:17:SER:CB	1:f:100:ARG:NH2	2.82	0.43
1:g:22:ILE:CD1	1:g:52:MET:HA	2.48	0.43
1:n:74:ILE:HD13	1:n:74:ILE:HG21	1.70	0.43
1:s:149:TYR:CD2	1:s:149:TYR:C	2.95	0.43
1:u:107:MET:SD	1:u:107:MET:C	3.02	0.43
2:C:200:HEM:HHB	2:C:200:HEM:HMA2	1.62	0.43
1:D:51:GLU:OE1	1:D:51:GLU:HA	2.19	0.43
1:G:30:LYS:HD2	1:G:30:LYS:HA	1.69	0.43
1:I:17:SER:CB	1:I:100:ARG:NH2	2.82	0.43
1:M:78:ARG:HB2	1:M:89:ALA:HB1	2.01	0.43
1:c:52:MET:HE2	2:c:200:HEM:C1C	2.53	0.43
1:f:17:SER:HB2	1:f:100:ARG:NH2	2.34	0.43
1:g:83:LEU:HB2	3:g:327:HOH:O	2.17	0.43
1:h:123:ILE:O	1:h:127:GLU:HG2	2.18	0.43
1:i:113:ASP:CG	1:i:116:SER:HB2	2.43	0.43
1:m:33:ASP:OD1	1:m:38:THR:HG22	2.19	0.43
1:o:51:GLU:OE1	1:o:51:GLU:HA	2.19	0.43
1:N:7:VAL:O	1:N:11:LEU:HG	2.19	0.42
1:g:84:ARG:NE	1:g:146:GLU:OE2	2.50	0.42
2:q:200:HEM:CHB	1:r:52:MET:HB3	2.49	0.42
1:C:64:LEU:C	1:C:64:LEU:HD23	2.45	0.42
1:M:77:LEU:HD13	1:N:72:GLN:OE1	2.19	0.42
1:N:120:LEU:HD23	1:N:120:LEU:HA	1.86	0.42
1:Q:140:LEU:O	1:Q:144:LEU:HG	2.20	0.42
2:R:200:HEM:HAD1	3:R:393:HOH:O	2.20	0.42
1:d:114:THR:O	1:d:118:VAL:HG23	2.19	0.42
1:e:28:HIS:CD2	1:e:86:GLN:HG2	2.55	0.42
1:j:90:ASP:O	1:j:94:GLU:HG2	2.19	0.42
1:m:68:LEU:HD23	3:m:227:HOH:O	2.19	0.42
1:s:52:MET:HG2	2:t:200:HEM:C4B	2.55	0.42
2:t:200:HEM:HBC2	2:t:200:HEM:CHD	2.25	0.42
1:x:12:ASN:HD21	1:x:70:ASN:N	2.15	0.42
1:F:40:LEU:HB2	1:F:153:CYS:HB3	2.00	0.42
1:F:61:ARG:NH1	1:F:64:LEU:HD22	2.34	0.42
1:G:159:THR:HG21	3:G:232:HOH:O	2.13	0.42
1:H:78:ARG:NH1	1:H:92:ALA:CB	2.82	0.42
1:a:4:ASP:HB3	1:a:7:VAL:HG23	2.01	0.42
1:h:51:GLU:OE2	1:h:51:GLU:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:53:ARG:CZ	3:h:249:HOH:O	2.66	0.42
1:i:24:GLN:OE1	3:i:281:HOH:O	2.21	0.42
1:k:102:LYS:CB	1:k:103:PRO:CD	2.97	0.42
1:l:33:ASP:OD1	1:l:38:THR:HG22	2.20	0.42
1:m:134:LEU:HD21	3:m:245:HOH:O	2.19	0.42
1:o:60:ASP:OD2	1:p:30:LYS:HE3	2.19	0.42
1:o:90:ASP:O	1:o:93:ILE:HG22	2.19	0.42
1:q:117:ALA:O	1:q:121:GLU:HG3	2.20	0.42
1:w:13:GLU:OE2	1:w:100:ARG:CD	2.67	0.42
1:C:61:ARG:CZ	1:C:115:THR:HB	2.49	0.42
1:N:25:TYR:OH	1:N:94:GLU:OE1	2.34	0.42
1:O:60:ASP:OD1	1:P:30:LYS:HE3	2.19	0.42
1:R:49:PHE:CE2	2:R:200:HEM:C3D	3.08	0.42
1:V:25:TYR:N	1:V:25:TYR:CD1	2.86	0.42
1:d:68:LEU:HB3	3:d:255:HOH:O	2.18	0.42
1:e:18:GLU:OE2	1:e:18:GLU:HA	2.20	0.42
2:e:200:HEM:NC	1:f:52:MET:HE2	2.34	0.42
1:g:33:ASP:HB3	3:g:334:HOH:O	2.18	0.42
1:o:102:LYS:HG2	3:q:384:HOH:O	2.20	0.42
1:q:52:MET:HE2	2:q:200:HEM:C4B	2.54	0.42
1:w:30:LYS:HB3	1:w:30:LYS:HE3	1.66	0.42
1:F:156:ARG:HA	1:F:157:PRO:HA	1.93	0.42
1:L:52:MET:HB3	2:L:200:HEM:C1D	2.54	0.42
2:S:200:HEM:CHB	1:T:52:MET:HB3	2.49	0.42
1:a:22:ILE:CD1	1:a:52:MET:HA	2.49	0.42
1:k:28:HIS:NE2	1:k:86:GLN:HG2	2.35	0.42
1:o:146:GLU:OE1	3:o:356:HOH:O	2.21	0.42
1:s:4:ASP:HA	1:s:5:PRO:HD3	1.88	0.42
1:w:94:GLU:O	1:w:95:TYR:C	2.60	0.42
1:A:28:HIS:CE1	1:A:86:GLN:HG2	2.54	0.42
1:E:4:ASP:HA	1:E:5:PRO:HD3	1.85	0.42
1:I:39:GLU:HB3	1:L:157:PRO:HD3	2.00	0.42
1:K:79:ILE:HD12	1:K:79:ILE:HG23	1.79	0.42
1:P:17:SER:HB2	1:P:100:ARG:NH2	2.35	0.42
1:P:107:MET:SD	1:P:107:MET:C	3.02	0.42
1:V:84:ARG:CD	3:V:306:HOH:O	2.67	0.42
1:W:18:GLU:OE2	1:W:18:GLU:HA	2.20	0.42
1:a:120:LEU:HD23	1:a:120:LEU:HA	1.86	0.42
1:c:26:PHE:CE2	1:c:30:LYS:HD3	2.53	0.42
1:g:91:LEU:HG	1:g:134:LEU:HD13	2.01	0.42
1:g:150:SER:O	1:g:153:CYS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:93:ILE:HG13	3:i:323:HOH:O	2.20	0.42
1:m:61:ARG:HD2	1:m:61:ARG:HA	1.80	0.42
1:q:1:MET:N	3:q:309:HOH:O	2.53	0.42
1:C:71:TYR:CE1	2:C:200:HEM:HBB1	2.54	0.42
1:C:124:VAL:O	1:C:128:GLU:HG3	2.19	0.42
2:C:200:HEM:C2D	1:D:52:MET:HB3	2.55	0.42
1:E:64:LEU:HD23	1:E:64:LEU:C	2.45	0.42
1:F:1:MET:HE2	1:W:131:ILE:HG22	2.02	0.42
2:I:200:HEM:HHD	2:I:200:HEM:CBC	2.45	0.42
1:N:94:GLU:O	1:N:97:VAL:N	2.46	0.42
3:a:302:HOH:O	1:v:102:LYS:HE3	2.19	0.42
1:k:61:ARG:NH2	1:k:115:THR:HB	2.35	0.42
1:m:91:LEU:HD22	1:m:95:TYR:HE2	1.84	0.42
1:o:156:ARG:HD3	3:o:367:HOH:O	2.09	0.42
1:w:141:MET:HE2	1:w:146:GLU:HG3	2.02	0.42
1:B:94:GLU:OE1	1:B:127:GLU:OE1	2.37	0.42
1:C:30:LYS:HA	1:C:30:LYS:HD2	1.87	0.42
1:C:78:ARG:NH1	1:C:92:ALA:HB1	2.35	0.42
1:E:48:SER:O	1:E:52:MET:HG3	2.20	0.42
1:G:148:LEU:HA	1:S:148:LEU:HD21	2.02	0.42
1:K:52:MET:HB3	2:L:200:HEM:CHB	2.50	0.42
1:K:124:VAL:O	1:K:128:GLU:HG3	2.20	0.42
1:P:21:ALA:O	1:P:22:ILE:C	2.62	0.42
1:S:1:MET:HE3	1:S:64:LEU:HD21	2.02	0.42
1:b:93:ILE:O	1:b:93:ILE:HG13	2.20	0.42
1:e:17:SER:CA	3:e:387:HOH:O	2.68	0.42
1:f:4:ASP:HA	1:f:5:PRO:HD3	1.87	0.42
1:v:101:LEU:HD22	1:v:120:LEU:HD22	2.02	0.42
1:x:125:ALA:O	3:x:384:HOH:O	2.21	0.42
1:B:73:ARG:HH11	1:e:73:ARG:NE	2.17	0.42
1:C:39:GLU:OE2	1:C:39:GLU:N	2.53	0.42
1:F:4:ASP:HA	1:F:5:PRO:HD2	1.82	0.42
1:J:64:LEU:C	1:J:64:LEU:HD23	2.45	0.42
1:J:139:GLU:HG2	3:J:248:HOH:O	2.20	0.42
1:O:78:ARG:HB2	1:O:89:ALA:HB1	2.02	0.42
1:Q:156:ARG:HA	1:Q:157:PRO:HA	1.87	0.42
1:b:149:TYR:CE1	1:c:158:PRO:HG2	2.54	0.42
1:A:102:LYS:HB3	1:T:112:GLN:OE1	2.20	0.42
1:J:156:ARG:HA	1:J:157:PRO:HA	1.85	0.42
1:K:4:ASP:OD2	1:K:6:ASP:HB2	2.20	0.42
1:N:93:ILE:O	1:N:94:GLU:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:138:LEU:O	1:O:141:MET:HB2	2.19	0.42
2:R:200:HEM:CAD	3:R:393:HOH:O	2.68	0.42
1:T:39:GLU:OE2	1:T:155:SER:HB3	2.20	0.42
1:d:81:GLN:H	1:d:85:GLU:CD	2.27	0.42
1:i:14:GLN:O	1:i:17:SER:HB3	2.19	0.42
2:k:200:HEM:HBD1	3:l:286:HOH:O	2.19	0.42
1:n:27:LEU:HD12	1:n:27:LEU:O	2.20	0.42
1:B:102:LYS:HB2	1:B:103:PRO:HD3	2.02	0.41
1:C:70:ASN:C	1:C:70:ASN:HD22	2.28	0.41
1:C:156:ARG:HA	1:C:157:PRO:HA	1.91	0.41
3:E:304:HOH:O	1:F:30:LYS:CE	2.67	0.41
1:G:78:ARG:HB3	1:G:89:ALA:HB1	2.02	0.41
1:H:4:ASP:HB3	1:H:7:VAL:HG23	2.01	0.41
1:P:83:LEU:HD23	1:P:83:LEU:HA	1.76	0.41
1:T:102:LYS:HB2	1:T:103:PRO:CD	2.50	0.41
1:U:156:ARG:HH11	1:U:156:ARG:HD3	1.68	0.41
1:d:107:MET:O	1:d:110:GLU:HB2	2.20	0.41
1:f:94:GLU:HB3	1:f:131:ILE:HD11	2.01	0.41
1:p:4:ASP:OD2	1:p:6:ASP:N	2.53	0.41
1:t:152:GLN:NE2	1:x:156:ARG:NH2	2.66	0.41
1:v:155:SER:OG	1:v:157:PRO:O	2.38	0.41
1:B:9:ARG:HH11	1:B:9:ARG:HG3	1.85	0.41
1:I:30:LYS:O	3:I:426:HOH:O	2.21	0.41
1:K:53:ARG:CG	3:L:373:HOH:O	2.66	0.41
2:R:200:HEM:HBB2	2:R:200:HEM:CHC	2.46	0.41
1:W:82:THR:O	1:W:83:LEU:C	2.62	0.41
1:i:19:LEU:HD11	1:i:71:TYR:HA	2.02	0.41
1:i:135:GLU:HB2	3:i:277:HOH:O	2.18	0.41
1:s:97:VAL:HG11	1:s:127:GLU:HG3	2.02	0.41
1:D:22:ILE:HD11	1:D:52:MET:HA	2.02	0.41
1:I:156:ARG:HA	1:I:157:PRO:HA	1.88	0.41
1:M:156:ARG:HA	1:M:157:PRO:HA	1.71	0.41
1:O:156:ARG:HA	1:O:157:PRO:HA	1.92	0.41
1:Q:102:LYS:HB2	1:Q:103:PRO:HD3	2.01	0.41
1:e:18:GLU:OE2	1:e:51:GLU:OE2	2.38	0.41
1:e:18:GLU:O	1:e:22:ILE:HG13	2.21	0.41
1:e:147:GLU:CD	1:e:147:GLU:N	2.78	0.41
1:f:78:ARG:NH2	3:f:245:HOH:O	2.52	0.41
1:h:94:GLU:CD	1:h:127:GLU:OE1	2.63	0.41
1:l:120:LEU:HD23	1:l:120:LEU:HA	1.85	0.41
1:m:149:TYR:CD2	1:m:149:TYR:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:37:PHE:HE1	1:o:150:SER:HB3	1.85	0.41
1:r:143:LYS:NZ	3:r:265:HOH:O	2.22	0.41
1:B:158:PRO:HG2	1:V:149:TYR:CE1	2.55	0.41
1:D:27:LEU:HD23	1:D:79:ILE:CD1	2.50	0.41
1:E:49:PHE:HB3	1:E:53:ARG:HH12	1.84	0.41
1:G:47:GLU:O	1:G:50:ASP:HB2	2.20	0.41
1:K:94:GLU:OE2	1:K:127:GLU:OE1	2.39	0.41
1:Q:40:LEU:CB	1:Q:153:CYS:HB3	2.50	0.41
2:X:200:HEM:HBB2	2:X:200:HEM:CHC	2.26	0.41
1:d:51:GLU:OE2	1:d:51:GLU:HA	2.20	0.41
1:f:1:MET:HE2	1:w:131:ILE:CG2	2.50	0.41
1:j:147:GLU:CD	1:j:147:GLU:H	2.29	0.41
1:k:1:MET:HE1	1:k:64:LEU:HD21	1.97	0.41
1:o:37:PHE:CE1	1:o:150:SER:HB3	2.56	0.41
1:p:98:LEU:HD22	1:p:124:VAL:HG13	2.01	0.41
1:t:64:LEU:HD23	1:t:64:LEU:O	2.18	0.41
1:D:18:GLU:OE2	1:D:18:GLU:HA	2.21	0.41
1:K:113:ASP:CB	3:K:239:HOH:O	2.62	0.41
1:M:147:GLU:N	1:M:147:GLU:CD	2.78	0.41
1:T:12:ASN:ND2	1:T:70:ASN:H	2.18	0.41
1:V:94:GLU:CG	3:V:273:HOH:O	2.69	0.41
1:c:91:LEU:HD21	1:c:135:GLU:HG3	2.03	0.41
1:c:113:ASP:OD2	1:c:116:SER:OG	2.22	0.41
1:h:18:GLU:OE2	1:h:18:GLU:HA	2.21	0.41
1:j:25:TYR:N	1:j:25:TYR:HD1	2.16	0.41
1:m:91:LEU:HD11	1:m:135:GLU:HG2	2.01	0.41
1:q:52:MET:HE2	2:q:200:HEM:NB	2.33	0.41
1:s:19:LEU:HD22	2:t:200:HEM:HBB1	2.01	0.41
1:B:63:LEU:HA	1:B:63:LEU:HD23	1.78	0.41
1:I:17:SER:HB2	1:I:100:ARG:NH2	2.35	0.41
1:J:158:PRO:HB2	1:X:137:GLN:OE1	2.20	0.41
1:M:52:MET:HG2	2:M:200:HEM:C1C	2.55	0.41
1:M:87:PHE:HE2	1:M:141:MET:HE3	1.86	0.41
1:M:147:GLU:CD	1:M:147:GLU:H	2.27	0.41
1:Q:4:ASP:HA	1:Q:5:PRO:HD3	1.91	0.41
1:R:40:LEU:CB	1:R:153:CYS:HB3	2.51	0.41
1:S:107:MET:HE2	1:S:108:CYS:HA	2.01	0.41
1:m:71:TYR:CD2	1:n:27:LEU:HD22	2.55	0.41
1:m:79:ILE:N	1:m:79:ILE:HD13	2.36	0.41
1:o:18:GLU:O	1:o:22:ILE:HG13	2.20	0.41
1:o:33:ASP:OD1	1:o:38:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:91:LEU:CD2	1:u:131:ILE:HG23	2.51	0.41
1:x:91:LEU:HD21	1:x:134:LEU:HB2	2.03	0.41
1:G:4:ASP:CB	1:G:7:VAL:HG23	2.44	0.41
1:H:159:THR:CG2	3:H:360:HOH:O	2.68	0.41
2:L:200:HEM:HBD2	2:L:200:HEM:CHA	2.50	0.41
1:S:30:LYS:HA	1:S:30:LYS:HD2	1.67	0.41
1:T:48:SER:O	1:T:52:MET:HG3	2.21	0.41
1:U:4:ASP:CG	1:U:7:VAL:HG23	2.46	0.41
1:d:78:ARG:C	1:d:79:ILE:HD13	2.46	0.41
3:d:235:HOH:O	1:m:112:GLN:HG2	2.21	0.41
1:l:21:ALA:HB2	1:l:93:ILE:CD1	2.50	0.41
1:p:149:TYR:CD2	1:p:149:TYR:C	2.98	0.41
1:q:20:THR:OG1	1:q:75:GLY:HA3	2.21	0.41
1:s:91:LEU:HD21	1:s:135:GLU:HG3	2.03	0.41
1:t:84:ARG:O	1:t:88:GLU:HG3	2.20	0.41
1:u:61:ARG:NH1	1:u:64:LEU:HD22	2.36	0.41
1:u:137:GLN:HE22	1:x:158:PRO:HB2	1.86	0.41
1:w:82:THR:O	1:w:83:LEU:C	2.60	0.41
1:B:123:ILE:O	1:B:127:GLU:HG2	2.21	0.41
1:D:4:ASP:CG	1:D:5:PRO:HD2	2.45	0.41
1:G:159:THR:HG21	3:G:217:HOH:O	2.19	0.41
1:M:17:SER:OG	1:M:100:ARG:NH2	2.54	0.41
1:R:113:ASP:CG	1:R:116:SER:HB2	2.46	0.41
1:a:18:GLU:OE2	1:a:18:GLU:HA	2.20	0.41
1:k:74:ILE:HD11	1:k:77:LEU:CD1	2.49	0.41
1:t:18:GLU:O	1:t:22:ILE:HG13	2.20	0.41
1:t:64:LEU:C	1:t:64:LEU:CD2	2.88	0.41
1:D:88:GLU:CG	3:D:216:HOH:O	2.37	0.41
1:F:27:LEU:HD12	1:F:31:MET:HG3	2.02	0.41
1:G:147:GLU:H	1:G:147:GLU:CD	2.29	0.41
1:H:156:ARG:HA	1:H:157:PRO:HA	1.85	0.41
1:M:17:SER:HB2	1:M:100:ARG:NH2	2.36	0.41
1:M:18:GLU:OE1	1:M:51:GLU:OE1	2.39	0.41
1:M:91:LEU:HD11	1:M:135:GLU:HG2	2.03	0.41
1:P:64:LEU:HD23	1:P:64:LEU:C	2.46	0.41
1:T:127:GLU:CD	3:T:282:HOH:O	2.64	0.41
1:T:131:ILE:O	1:T:135:GLU:HG3	2.21	0.41
1:U:97:VAL:HG11	1:U:127:GLU:HG3	2.01	0.41
1:X:18:GLU:OE2	1:X:51:GLU:OE2	2.38	0.41
1:c:4:ASP:HA	1:c:5:PRO:HD3	1.82	0.41
1:i:91:LEU:HD21	1:i:135:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:l:226:HOH:O	1:q:102:LYS:HE3	2.21	0.41
1:s:52:MET:HE2	2:t:200:HEM:C4C	2.55	0.41
1:A:94:GLU:OE1	1:A:131:ILE:HG13	2.20	0.41
1:G:102:LYS:CB	1:G:103:PRO:CD	2.84	0.41
1:G:154:VAL:CG2	1:G:158:PRO:HG3	2.51	0.41
1:O:158:PRO:HD2	3:O:255:HOH:O	2.20	0.41
1:R:47:GLU:HA	1:R:47:GLU:OE1	2.20	0.41
1:b:107:MET:O	1:b:111:LYS:HG2	2.21	0.41
1:f:156:ARG:HA	1:f:157:PRO:HA	1.76	0.41
1:i:85:GLU:HG2	3:i:317:HOH:O	2.19	0.41
2:q:200:HEM:HMC2	2:q:200:HEM:CBC	2.43	0.41
1:s:30:LYS:HA	1:s:30:LYS:HD2	1.94	0.41
1:t:141:MET:CE	1:t:146:GLU:OE1	2.69	0.41
1:w:49:PHE:CE2	2:x:200:HEM:C4D	3.09	0.41
1:w:102:LYS:HG3	1:w:102:LYS:H	1.73	0.41
1:D:58:ILE:HD13	1:D:58:ILE:HG21	1.82	0.40
1:F:122:LYS:HD2	3:F:383:HOH:O	2.20	0.40
1:K:2:GLN:HE21	1:K:66:ASP:HB3	1.86	0.40
1:Q:149:TYR:CD2	1:Q:149:TYR:C	2.99	0.40
1:R:1:MET:CA	3:R:330:HOH:O	2.68	0.40
1:T:22:ILE:HD11	1:T:52:MET:HA	2.02	0.40
1:X:22:ILE:HG13	1:X:51:GLU:HB3	2.03	0.40
1:f:94:GLU:OE1	1:f:127:GLU:OE1	2.38	0.40
1:t:11:LEU:HA	1:t:11:LEU:HD23	1.71	0.40
1:v:107:MET:O	1:v:108:CYS:C	2.63	0.40
1:x:11:LEU:HA	1:x:11:LEU:HD23	1.46	0.40
1:E:19:LEU:HA	1:E:22:ILE:HD12	2.01	0.40
1:E:50:ASP:OD2	1:E:53:ARG:NH2	2.54	0.40
1:F:94:GLU:OE2	1:F:130:HIS:CD2	2.74	0.40
1:G:27:LEU:HD23	1:G:79:ILE:HD12	2.02	0.40
1:I:37:PHE:CD2	1:I:83:LEU:HD21	2.56	0.40
1:M:77:LEU:HD13	1:N:72:GLN:CD	2.46	0.40
1:u:18:GLU:OE1	1:u:18:GLU:HA	2.22	0.40
1:w:4:ASP:HA	1:w:5:PRO:HD3	1.83	0.40
1:Q:148:LEU:HA	1:Q:148:LEU:HD12	1.83	0.40
1:S:107:MET:CE	1:S:107:MET:C	2.95	0.40
1:W:54:HIS:O	1:W:58:ILE:HG13	2.21	0.40
1:a:61:ARG:HA	1:a:61:ARG:HD2	1.95	0.40
1:a:94:GLU:OE2	1:a:127:GLU:OE1	2.40	0.40
1:d:133:TYR:O	1:d:137:GLN:HG2	2.21	0.40
1:k:91:LEU:HD23	1:k:91:LEU:HA	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:s:52:MET:CE	2:t:200:HEM:C4C	3.04	0.40
1:v:107:MET:C	1:v:107:MET:SD	3.04	0.40
1:w:50:ASP:OD1	1:w:53:ARG:NH2	2.54	0.40
1:w:78:ARG:NH1	1:w:92:ALA:HB1	2.37	0.40
1:x:55:ALA:HB3	2:x:200:HEM:CBC	2.50	0.40
1:J:137:GLN:OE1	1:T:158:PRO:HB2	2.21	0.40
1:R:26:PHE:CD1	2:R:200:HEM:HAC	2.56	0.40
1:k:14:GLN:O	1:k:15:LEU:C	2.64	0.40
1:n:53:ARG:O	1:n:57:GLU:HG3	2.21	0.40
1:p:50:ASP:HA	1:p:53:ARG:NH2	2.36	0.40
1:q:52:MET:CE	2:q:200:HEM:C1B	3.04	0.40
1:C:94:GLU:OE2	1:C:127:GLU:OE1	2.39	0.40
1:F:19:LEU:HD23	1:F:22:ILE:HD12	2.03	0.40
1:G:27:LEU:HD23	1:G:79:ILE:CD1	2.52	0.40
1:I:46:ALA:HB3	3:I:335:HOH:O	2.22	0.40
1:L:61:ARG:NH2	1:L:115:THR:HB	2.37	0.40
1:R:49:PHE:CE2	2:R:200:HEM:C4D	3.09	0.40
2:e:200:HEM:NC	1:f:52:MET:CE	2.85	0.40
2:g:200:HEM:CHD	2:g:200:HEM:CBC	2.94	0.40
1:x:140:LEU:HD23	1:x:140:LEU:HA	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
1	B	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	C	157/161 (98%)	157 (100%)	0	0	100	100
1	D	157/161 (98%)	156 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	157/161 (98%)	157 (100%)	0	0	100	100
1	F	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	G	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	H	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	I	157/161 (98%)	157 (100%)	0	0	100	100
1	J	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	K	157/161 (98%)	157 (100%)	0	0	100	100
1	L	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	M	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	N	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	O	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	P	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	Q	157/161 (98%)	157 (100%)	0	0	100	100
1	R	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	S	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	T	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	U	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	V	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	W	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	X	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	a	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	b	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	c	157/161 (98%)	157 (100%)	0	0	100	100
1	d	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
1	e	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	f	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	g	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	h	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	i	157/161 (98%)	157 (100%)	0	0	100	100
1	j	157/161 (98%)	157 (100%)	0	0	100	100
1	k	157/161 (98%)	157 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	l	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	m	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
1	n	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	o	157/161 (98%)	157 (100%)	0	0	100	100
1	p	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	q	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
1	r	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
1	s	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	t	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	u	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	v	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	w	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
1	x	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
All	All	7536/7728 (98%)	7492 (99%)	44 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	142/143 (99%)	139 (98%)	3 (2%)	47	44
1	B	142/143 (99%)	138 (97%)	4 (3%)	38	32
1	C	142/143 (99%)	136 (96%)	6 (4%)	26	19
1	D	142/143 (99%)	138 (97%)	4 (3%)	38	32
1	E	142/143 (99%)	134 (94%)	8 (6%)	19	11
1	F	142/143 (99%)	137 (96%)	5 (4%)	32	24
1	G	142/143 (99%)	139 (98%)	3 (2%)	47	44
1	H	142/143 (99%)	137 (96%)	5 (4%)	32	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	142/143 (99%)	137 (96%)	5 (4%)	32	24
1	J	142/143 (99%)	135 (95%)	7 (5%)	22	14
1	K	142/143 (99%)	136 (96%)	6 (4%)	26	19
1	L	142/143 (99%)	140 (99%)	2 (1%)	59	59
1	M	142/143 (99%)	135 (95%)	7 (5%)	22	14
1	N	142/143 (99%)	135 (95%)	7 (5%)	22	14
1	O	142/143 (99%)	140 (99%)	2 (1%)	59	59
1	P	142/143 (99%)	139 (98%)	3 (2%)	47	44
1	Q	142/143 (99%)	137 (96%)	5 (4%)	32	24
1	R	142/143 (99%)	138 (97%)	4 (3%)	38	32
1	S	142/143 (99%)	137 (96%)	5 (4%)	32	24
1	T	142/143 (99%)	134 (94%)	8 (6%)	19	11
1	U	142/143 (99%)	137 (96%)	5 (4%)	32	24
1	V	142/143 (99%)	136 (96%)	6 (4%)	26	19
1	W	142/143 (99%)	135 (95%)	7 (5%)	22	14
1	X	142/143 (99%)	139 (98%)	3 (2%)	47	44
1	a	142/143 (99%)	136 (96%)	6 (4%)	26	19
1	b	142/143 (99%)	138 (97%)	4 (3%)	38	32
1	c	142/143 (99%)	138 (97%)	4 (3%)	38	32
1	d	142/143 (99%)	138 (97%)	4 (3%)	38	32
1	e	142/143 (99%)	138 (97%)	4 (3%)	38	32
1	f	142/143 (99%)	141 (99%)	1 (1%)	76	78
1	g	142/143 (99%)	138 (97%)	4 (3%)	38	32
1	h	142/143 (99%)	136 (96%)	6 (4%)	26	19
1	i	142/143 (99%)	140 (99%)	2 (1%)	59	59
1	j	142/143 (99%)	138 (97%)	4 (3%)	38	32
1	k	142/143 (99%)	135 (95%)	7 (5%)	22	14
1	l	142/143 (99%)	141 (99%)	1 (1%)	76	78
1	m	141/143 (99%)	132 (94%)	9 (6%)	16	8
1	n	142/143 (99%)	135 (95%)	7 (5%)	22	14
1	o	142/143 (99%)	140 (99%)	2 (1%)	59	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	p	141/143 (99%)	136 (96%)	5 (4%)	32	24
1	q	142/143 (99%)	137 (96%)	5 (4%)	32	24
1	r	142/143 (99%)	138 (97%)	4 (3%)	38	32
1	s	142/143 (99%)	140 (99%)	2 (1%)	59	59
1	t	142/143 (99%)	138 (97%)	4 (3%)	38	32
1	u	142/143 (99%)	136 (96%)	6 (4%)	26	19
1	v	142/143 (99%)	134 (94%)	8 (6%)	19	11
1	w	142/143 (99%)	136 (96%)	6 (4%)	26	19
1	x	142/143 (99%)	138 (97%)	4 (3%)	38	32
All	All	6814/6864 (99%)	6585 (97%)	229 (3%)	32	25

All (229) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	GLU
1	A	77	LEU
1	A	159	THR
1	B	18	GLU
1	B	51	GLU
1	B	53	ARG
1	B	73	ARG
1	C	9	ARG
1	C	39	GLU
1	C	77	LEU
1	C	93	ILE
1	C	112	GLN
1	C	159	THR
1	D	2	GLN
1	D	93	ILE
1	D	106	VAL
1	D	159	THR
1	E	2	GLN
1	E	30	LYS
1	E	73	ARG
1	E	74	ILE
1	E	77	LEU
1	E	88	GLU
1	E	93	ILE
1	E	141	MET

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Mol	Chain	Res	Type
1	F	74	ILE
1	F	79	ILE
1	F	91	LEU
1	F	93	ILE
1	F	154	VAL
1	G	77	LEU
1	G	154	VAL
1	G	159	THR
1	H	61	ARG
1	H	74	ILE
1	H	93	ILE
1	H	137	GLN
1	H	159	THR
1	I	2	GLN
1	I	74	ILE
1	I	77	LEU
1	I	124	VAL
1	I	159	THR
1	J	1	MET
1	J	2	GLN
1	J	33	ASP
1	J	48	SER
1	J	77	LEU
1	J	93	ILE
1	J	159	THR
1	K	51	GLU
1	K	74	ILE
1	K	77	LEU
1	K	124	VAL
1	K	154	VAL
1	K	159	THR
1	L	88	GLU
1	L	159	THR
1	M	9	ARG
1	M	48	SER
1	M	76	SER
1	M	77	LEU
1	M	88	GLU
1	M	137	GLN
1	M	159	THR
1	N	4	ASP
1	N	74	ILE

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Mol	Chain	Res	Type
1	N	77	LEU
1	N	81	GLN
1	N	93	ILE
1	N	136	THR
1	N	154	VAL
1	O	74	ILE
1	O	154	VAL
1	P	77	LEU
1	P	78	ARG
1	P	159	THR
1	Q	2	GLN
1	Q	9	ARG
1	Q	74	ILE
1	Q	77	LEU
1	Q	159	THR
1	R	48	SER
1	R	119	LEU
1	R	127	GLU
1	R	159	THR
1	S	77	LEU
1	S	88	GLU
1	S	93	ILE
1	S	107	MET
1	S	159	THR
1	T	2	GLN
1	T	15	LEU
1	T	33	ASP
1	T	77	LEU
1	T	88	GLU
1	T	124	VAL
1	T	154	VAL
1	T	159	THR
1	U	2	GLN
1	U	77	LEU
1	U	110	GLU
1	U	127	GLU
1	U	159	THR
1	V	1	MET
1	V	2	GLN
1	V	39	GLU
1	V	48	SER
1	V	77	LEU

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Mol	Chain	Res	Type
1	V	102	LYS
1	W	29	SER
1	W	48	SER
1	W	51	GLU
1	W	74	ILE
1	W	77	LEU
1	W	78	ARG
1	W	93	ILE
1	X	2	GLN
1	X	137	GLN
1	X	154	VAL
1	a	2	GLN
1	a	15	LEU
1	a	30	LYS
1	a	137	GLN
1	a	142	ASP
1	a	159	THR
1	b	93	ILE
1	b	124	VAL
1	b	146	GLU
1	b	159	THR
1	c	66	ASP
1	c	77	LEU
1	c	91	LEU
1	c	159	THR
1	d	16	THR
1	d	79	ILE
1	d	156	ARG
1	d	159	THR
1	e	2	GLN
1	e	79	ILE
1	e	146	GLU
1	e	159	THR
1	f	20	THR
1	g	74	ILE
1	g	76	SER
1	g	77	LEU
1	g	159	THR
1	h	2	GLN
1	h	9	ARG
1	h	74	ILE
1	h	110	GLU

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Mol	Chain	Res	Type
1	h	154	VAL
1	h	159	THR
1	i	1	MET
1	i	2	GLN
1	j	2	GLN
1	j	77	LEU
1	j	93	ILE
1	j	159	THR
1	k	2	GLN
1	k	74	ILE
1	k	77	LEU
1	k	79	ILE
1	k	88	GLU
1	k	93	ILE
1	k	102	LYS
1	l	1	MET
1	m	2	GLN
1	m	61	ARG
1	m	66	ASP
1	m	74	ILE
1	m	79	ILE
1	m	91	LEU
1	m	102	LYS
1	m	124	VAL
1	m	159	THR
1	n	4	ASP
1	n	30	LYS
1	n	33	ASP
1	n	76	SER
1	n	77	LEU
1	n	154	VAL
1	n	159	THR
1	o	74	ILE
1	o	77	LEU
1	p	66	ASP
1	p	74	ILE
1	p	77	LEU
1	p	93	ILE
1	p	100	ARG
1	q	51	GLU
1	q	74	ILE
1	q	77	LEU

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Mol	Chain	Res	Type
1	q	110	GLU
1	q	146	GLU
1	r	17	SER
1	r	100	ARG
1	r	137	GLN
1	r	159	THR
1	s	77	LEU
1	s	159	THR
1	t	9	ARG
1	t	51	GLU
1	t	93	ILE
1	t	101	LEU
1	u	1	MET
1	u	77	LEU
1	u	106	VAL
1	u	154	VAL
1	u	156	ARG
1	u	159	THR
1	v	29	SER
1	v	51	GLU
1	v	74	ILE
1	v	77	LEU
1	v	93	ILE
1	v	115	THR
1	v	152	GLN
1	v	159	THR
1	w	2	GLN
1	w	38	THR
1	w	68	LEU
1	w	76	SER
1	w	77	LEU
1	w	141	MET
1	x	2	GLN
1	x	77	LEU
1	x	93	ILE
1	x	119	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	43	HIS

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Mol	Chain	Res	Type
1	A	99	ASN
1	B	12	ASN
1	B	43	HIS
1	C	70	ASN
1	C	99	ASN
1	D	112	GLN
1	E	43	HIS
1	F	43	HIS
1	F	99	ASN
1	G	43	HIS
1	H	137	GLN
1	I	43	HIS
1	I	86	GLN
1	J	81	GLN
1	K	2	GLN
1	K	81	GLN
1	L	70	ASN
1	L	130	HIS
1	M	54	HIS
1	M	137	GLN
1	N	32	GLN
1	N	43	HIS
1	N	130	HIS
1	O	43	HIS
1	Q	81	GLN
1	Q	99	ASN
1	R	23	ASN
1	R	86	GLN
1	S	43	HIS
1	T	12	ASN
1	T	24	GLN
1	T	99	ASN
1	U	24	GLN
1	U	86	GLN
1	U	99	ASN
1	V	70	ASN
1	V	81	GLN
1	V	99	ASN
1	W	24	GLN
1	X	112	GLN
1	a	130	HIS
1	d	14	GLN

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Mol	Chain	Res	Type
1	d	137	GLN
1	d	152	GLN
1	e	14	GLN
1	e	34	ASN
1	e	72	GLN
1	e	112	GLN
1	f	24	GLN
1	f	112	GLN
1	f	130	HIS
1	g	43	HIS
1	h	14	GLN
1	h	32	GLN
1	h	43	HIS
1	h	54	HIS
1	i	32	GLN
1	k	99	ASN
1	k	137	GLN
1	l	32	GLN
1	l	81	GLN
1	m	24	GLN
1	n	43	HIS
1	o	32	GLN
1	o	34	ASN
1	o	112	GLN
1	p	152	GLN
1	q	24	GLN
1	q	86	GLN
1	q	112	GLN
1	r	86	GLN
1	t	24	GLN
1	t	70	ASN
1	t	99	ASN
1	t	130	HIS
1	t	152	GLN
1	u	112	GLN
1	u	137	GLN
1	u	152	GLN
1	v	99	ASN
1	v	112	GLN
1	v	137	GLN
1	w	2	GLN
1	w	34	ASN

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Mol	Chain	Res	Type
1	w	70	ASN
1	x	12	ASN
1	x	24	GLN
1	x	99	ASN
1	x	152	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	t	200	1	50,50,50	2.41	16 (32%)	67,82,82	1.72	17 (25%)
2	HEM	n	200	1	50,50,50	2.07	14 (28%)	67,82,82	1.50	14 (20%)
2	HEM	k	200	1	50,50,50	2.14	14 (28%)	67,82,82	1.57	15 (22%)
2	HEM	v	200	1	50,50,50	2.29	13 (26%)	67,82,82	2.25	28 (41%)
2	HEM	U	200	1	50,50,50	2.32	13 (26%)	67,82,82	2.11	18 (26%)
2	HEM	P	200	1	50,50,50	2.05	14 (28%)	67,82,82	1.77	16 (23%)
2	HEM	M	200	1	50,50,50	1.96	12 (24%)	67,82,82	1.68	16 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	C	200	1	50,50,50	3.54	19 (38%)	67,82,82	3.58	22 (32%)
2	HEM	g	200	1	50,50,50	2.27	13 (26%)	67,82,82	1.62	18 (26%)
2	HEM	B	200	1	50,50,50	2.18	12 (24%)	67,82,82	1.47	10 (14%)
2	HEM	q	200	1	50,50,50	2.12	13 (26%)	67,82,82	1.37	7 (10%)
2	HEM	I	200	1	50,50,50	2.46	17 (34%)	67,82,82	2.14	21 (31%)
2	HEM	e	200	1	50,50,50	2.11	10 (20%)	67,82,82	1.88	18 (26%)
2	HEM	F	200	1	50,50,50	2.29	12 (24%)	67,82,82	1.86	13 (19%)
2	HEM	o	200	1	50,50,50	2.29	14 (28%)	67,82,82	1.71	10 (14%)
2	HEM	L	200	1	50,50,50	2.33	13 (26%)	67,82,82	2.30	26 (38%)
2	HEM	c	200	1	50,50,50	1.98	10 (20%)	67,82,82	2.00	20 (29%)
2	HEM	x	200	1	50,50,50	2.65	13 (26%)	67,82,82	2.11	22 (32%)
2	HEM	S	200	1	50,50,50	2.06	19 (38%)	67,82,82	2.54	26 (38%)
2	HEM	H	200	1	50,50,50	2.15	9 (18%)	67,82,82	2.03	17 (25%)
2	HEM	X	200	1	50,50,50	2.71	14 (28%)	67,82,82	2.36	24 (35%)
2	HEM	R	200	1	50,50,50	2.46	14 (28%)	67,82,82	1.80	12 (17%)
2	HEM	a	200	1	50,50,50	2.56	12 (24%)	67,82,82	2.37	24 (35%)
2	HEM	j	200	1	50,50,50	1.97	15 (30%)	67,82,82	2.65	25 (37%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	t	200	1	-	11/14/54/54	-
2	HEM	n	200	1	-	2/14/54/54	-
2	HEM	k	200	1	-	10/14/54/54	-
2	HEM	v	200	1	-	8/14/54/54	-
2	HEM	U	200	1	-	4/14/54/54	-
2	HEM	P	200	1	-	5/14/54/54	-
2	HEM	M	200	1	-	8/14/54/54	-
2	HEM	C	200	1	-	8/14/54/54	-
2	HEM	g	200	1	-	6/14/54/54	-
2	HEM	B	200	1	-	3/14/54/54	-
2	HEM	q	200	1	-	4/14/54/54	-
2	HEM	I	200	1	-	3/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	e	200	1	-	6/14/54/54	-
2	HEM	F	200	1	-	6/14/54/54	-
2	HEM	o	200	1	-	8/14/54/54	-
2	HEM	L	200	1	-	8/14/54/54	-
2	HEM	c	200	1	-	7/14/54/54	-
2	HEM	x	200	1	-	5/14/54/54	-
2	HEM	S	200	1	-	4/14/54/54	-
2	HEM	H	200	1	-	6/14/54/54	-
2	HEM	X	200	1	-	7/14/54/54	-
2	HEM	R	200	1	-	10/14/54/54	-
2	HEM	a	200	1	-	1/14/54/54	-
2	HEM	j	200	1	-	2/14/54/54	-

All (325) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	200	HEM	FE-ND	-13.43	1.53	1.94
2	C	200	HEM	FE-NC	11.65	2.33	1.95
2	C	200	HEM	FE-NB	10.69	2.27	1.94
2	x	200	HEM	FE-NA	9.64	2.27	1.95
2	g	200	HEM	FE-NC	9.41	2.26	1.95
2	a	200	HEM	FE-ND	9.35	2.23	1.94
2	X	200	HEM	FE-NB	9.12	2.23	1.94
2	x	200	HEM	FE-ND	8.86	2.22	1.94
2	a	200	HEM	C3D-C2D	8.71	1.55	1.36
2	e	200	HEM	C3D-C2D	8.57	1.55	1.36
2	o	200	HEM	FE-NC	8.37	2.22	1.95
2	I	200	HEM	FE-NB	8.28	2.20	1.94
2	X	200	HEM	FE-NA	8.02	2.21	1.95
2	X	200	HEM	C3D-C2D	8.00	1.54	1.36
2	L	200	HEM	C3D-C2D	7.99	1.54	1.36
2	k	200	HEM	C3D-C2D	7.97	1.54	1.36
2	F	200	HEM	FE-NC	7.93	2.21	1.95
2	I	200	HEM	C3D-C2D	7.90	1.53	1.36
2	v	200	HEM	FE-NB	7.74	2.18	1.94
2	F	200	HEM	C3D-C2D	7.70	1.53	1.36
2	x	200	HEM	C3D-C2D	7.70	1.53	1.36
2	g	200	HEM	C3D-C2D	7.64	1.53	1.36
2	M	200	HEM	C3D-C2D	7.53	1.53	1.36
2	C	200	HEM	C3D-C2D	7.43	1.52	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	200	HEM	C3D-C2D	7.38	1.52	1.36
2	H	200	HEM	FE-NB	7.33	2.17	1.94
2	R	200	HEM	C3D-C2D	7.29	1.52	1.36
2	c	200	HEM	C3D-C2D	7.26	1.52	1.36
2	q	200	HEM	C3D-C2D	7.22	1.52	1.36
2	o	200	HEM	C3D-C2D	7.18	1.52	1.36
2	R	200	HEM	FE-ND	7.17	2.17	1.94
2	R	200	HEM	FE-NB	7.17	2.17	1.94
2	B	200	HEM	C3D-C2D	7.14	1.52	1.36
2	B	200	HEM	FE-NA	7.12	2.18	1.95
2	R	200	HEM	FE-NA	7.12	2.18	1.95
2	P	200	HEM	C3D-C2D	6.90	1.51	1.36
2	v	200	HEM	C3D-C2D	6.89	1.51	1.36
2	U	200	HEM	C3D-C2D	6.73	1.51	1.36
2	e	200	HEM	FE-NC	6.69	2.17	1.95
2	U	200	HEM	FE-NB	6.58	2.15	1.94
2	n	200	HEM	C3D-C2D	6.48	1.50	1.36
2	k	200	HEM	FE-NA	6.48	2.16	1.95
2	a	200	HEM	FE-NC	6.47	2.16	1.95
2	t	200	HEM	C3D-C2D	6.45	1.50	1.36
2	t	200	HEM	FE-NA	6.39	2.16	1.95
2	q	200	HEM	FE-NC	6.33	2.16	1.95
2	L	200	HEM	FE-NB	6.31	2.14	1.94
2	U	200	HEM	FE-NC	6.28	2.15	1.95
2	j	200	HEM	C3D-C2D	5.90	1.49	1.36
2	U	200	HEM	FE-ND	5.58	2.12	1.94
2	X	200	HEM	FE-ND	5.54	2.12	1.94
2	L	200	HEM	FE-NC	5.49	2.13	1.95
2	M	200	HEM	FE-NB	5.39	2.11	1.94
2	H	200	HEM	FE-ND	5.32	2.11	1.94
2	c	200	HEM	FE-NA	5.27	2.12	1.95
2	B	200	HEM	FE-NB	5.19	2.10	1.94
2	t	200	HEM	C4A-NA	-5.02	1.30	1.39
2	t	200	HEM	FE-ND	-4.98	1.79	1.94
2	S	200	HEM	C4C-NC	-4.91	1.30	1.39
2	t	200	HEM	C1A-NA	-4.87	1.30	1.39
2	H	200	HEM	FE-NC	4.82	2.11	1.95
2	L	200	HEM	FE-ND	4.80	2.09	1.94
2	P	200	HEM	FE-NA	-4.61	1.79	1.95
2	a	200	HEM	CMC-C2C	4.52	1.60	1.50
2	F	200	HEM	FE-NB	4.52	2.08	1.94
2	n	200	HEM	C3C-C2C	-4.44	1.28	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	200	HEM	FE-ND	4.22	2.07	1.94
2	k	200	HEM	C3B-C2B	-4.21	1.28	1.37
2	I	200	HEM	C3C-C2C	-4.18	1.28	1.37
2	I	200	HEM	FE-ND	4.15	2.07	1.94
2	X	200	HEM	FE-NC	4.15	2.08	1.95
2	I	200	HEM	C1B-NB	-4.14	1.33	1.40
2	L	200	HEM	CAC-C3C	4.14	1.58	1.47
2	B	200	HEM	FE-NC	4.11	2.08	1.95
2	n	200	HEM	FE-NC	4.11	2.08	1.95
2	v	200	HEM	C3B-C2B	-4.08	1.28	1.37
2	c	200	HEM	FE-NB	4.06	2.07	1.94
2	t	200	HEM	C3B-C2B	-4.05	1.28	1.37
2	L	200	HEM	FE-NA	3.99	2.08	1.95
2	o	200	HEM	FE-NB	3.98	2.07	1.94
2	q	200	HEM	FE-NA	3.92	2.08	1.95
2	j	200	HEM	C3C-C2C	-3.88	1.29	1.37
2	M	200	HEM	FE-ND	3.84	2.06	1.94
2	t	200	HEM	FE-NC	3.84	2.07	1.95
2	j	200	HEM	FE-ND	3.82	2.06	1.94
2	o	200	HEM	C3C-C2C	-3.75	1.29	1.37
2	a	200	HEM	FE-NB	3.73	2.06	1.94
2	S	200	HEM	FE-NC	3.71	2.07	1.95
2	g	200	HEM	FE-NA	3.70	2.07	1.95
2	P	200	HEM	C3B-C2B	-3.69	1.29	1.37
2	a	200	HEM	FE-NA	3.66	2.07	1.95
2	X	200	HEM	C1B-NB	-3.64	1.33	1.40
2	S	200	HEM	C3D-C2D	3.63	1.44	1.36
2	L	200	HEM	CMA-C3A	3.59	1.58	1.50
2	k	200	HEM	C3C-C2C	-3.59	1.29	1.37
2	U	200	HEM	C4D-ND	-3.59	1.34	1.40
2	U	200	HEM	C3B-C2B	-3.57	1.29	1.37
2	C	200	HEM	CHD-C4C	-3.56	1.31	1.38
2	C	200	HEM	C4C-NC	-3.55	1.32	1.39
2	t	200	HEM	C2A-C3A	-3.53	1.29	1.38
2	S	200	HEM	CAA-C2A	3.53	1.60	1.51
2	S	200	HEM	C1B-NB	-3.52	1.34	1.40
2	I	200	HEM	CAC-C3C	3.49	1.56	1.47
2	x	200	HEM	C3B-C2B	-3.49	1.30	1.37
2	j	200	HEM	C3B-C2B	-3.48	1.30	1.37
2	q	200	HEM	FE-NB	3.47	2.05	1.94
2	U	200	HEM	C3C-C2C	-3.46	1.30	1.37
2	S	200	HEM	CAB-C3B	3.44	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	200	HEM	C1B-NB	-3.42	1.34	1.40
2	v	200	HEM	C2A-C3A	-3.40	1.30	1.38
2	t	200	HEM	C3C-C2C	-3.40	1.30	1.37
2	j	200	HEM	C1B-NB	-3.40	1.34	1.40
2	v	200	HEM	C4A-NA	-3.40	1.33	1.39
2	n	200	HEM	C3B-C2B	-3.39	1.30	1.37
2	S	200	HEM	C3B-C2B	-3.38	1.30	1.37
2	U	200	HEM	C1B-NB	-3.38	1.34	1.40
2	o	200	HEM	FE-ND	3.37	2.05	1.94
2	R	200	HEM	C1B-NB	-3.35	1.34	1.40
2	X	200	HEM	CMB-C2B	3.34	1.57	1.50
2	F	200	HEM	C4C-NC	-3.32	1.33	1.39
2	x	200	HEM	C4A-NA	-3.32	1.33	1.39
2	c	200	HEM	FE-ND	3.31	2.05	1.94
2	C	200	HEM	CAB-C3B	3.29	1.56	1.47
2	B	200	HEM	CAB-C3B	3.28	1.56	1.47
2	x	200	HEM	C3C-C2C	-3.27	1.30	1.37
2	v	200	HEM	C3C-C2C	-3.26	1.30	1.37
2	a	200	HEM	C4A-NA	-3.24	1.33	1.39
2	k	200	HEM	C2A-C3A	-3.24	1.30	1.38
2	F	200	HEM	C3B-C2B	-3.23	1.30	1.37
2	e	200	HEM	FE-ND	3.22	2.04	1.94
2	v	200	HEM	C3C-C4C	-3.21	1.40	1.46
2	j	200	HEM	CAB-C3B	3.19	1.55	1.47
2	n	200	HEM	C1B-NB	-3.19	1.34	1.40
2	I	200	HEM	CMA-C3A	3.14	1.57	1.50
2	H	200	HEM	FE-NA	3.14	2.05	1.95
2	C	200	HEM	CMC-C2C	3.14	1.57	1.50
2	P	200	HEM	CAB-C3B	3.12	1.55	1.47
2	n	200	HEM	O2D-CGD	-3.09	1.20	1.30
2	v	200	HEM	C1B-NB	-3.09	1.34	1.40
2	I	200	HEM	FE-NA	-3.08	1.85	1.95
2	q	200	HEM	C1A-NA	-3.08	1.33	1.39
2	X	200	HEM	CMD-C2D	3.06	1.57	1.50
2	B	200	HEM	CMD-C2D	3.05	1.57	1.50
2	x	200	HEM	C4C-NC	-3.05	1.33	1.39
2	X	200	HEM	CAC-C3C	3.05	1.55	1.47
2	e	200	HEM	FE-NA	3.04	2.05	1.95
2	v	200	HEM	CAA-C2A	3.03	1.59	1.51
2	n	200	HEM	FE-NB	3.01	2.04	1.94
2	P	200	HEM	C2A-C3A	-3.00	1.31	1.38
2	C	200	HEM	C1D-ND	2.99	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	t	200	HEM	C4C-NC	-2.98	1.34	1.39
2	t	200	HEM	CHB-C4A	-2.97	1.32	1.39
2	g	200	HEM	C4C-NC	-2.95	1.34	1.39
2	n	200	HEM	CHA-C1A	-2.94	1.32	1.39
2	S	200	HEM	C3B-C4B	-2.92	1.39	1.44
2	L	200	HEM	CAB-C3B	2.91	1.55	1.47
2	q	200	HEM	C4C-NC	-2.91	1.34	1.39
2	S	200	HEM	C1A-NA	2.91	1.45	1.39
2	R	200	HEM	C4A-NA	-2.90	1.34	1.39
2	M	200	HEM	CAC-C3C	2.90	1.55	1.47
2	H	200	HEM	CMB-C2B	2.89	1.56	1.50
2	P	200	HEM	FE-ND	2.89	2.03	1.94
2	X	200	HEM	CAB-C3B	2.88	1.55	1.47
2	o	200	HEM	C2A-C3A	-2.88	1.31	1.38
2	c	200	HEM	CMB-C2B	2.87	1.56	1.50
2	o	200	HEM	C1A-NA	-2.85	1.34	1.39
2	I	200	HEM	C2A-C3A	-2.82	1.31	1.38
2	e	200	HEM	CAB-C3B	2.82	1.54	1.47
2	e	200	HEM	CMC-C2C	2.81	1.56	1.50
2	o	200	HEM	C1B-NB	-2.81	1.35	1.40
2	t	200	HEM	C1C-NC	-2.80	1.34	1.39
2	B	200	HEM	C4C-NC	-2.79	1.34	1.39
2	P	200	HEM	CMC-C2C	2.79	1.56	1.50
2	C	200	HEM	FE-NA	-2.78	1.86	1.95
2	j	200	HEM	CMC-C2C	2.77	1.56	1.50
2	k	200	HEM	CHB-C4A	-2.77	1.33	1.39
2	S	200	HEM	CAD-C3D	2.74	1.58	1.51
2	c	200	HEM	C3B-C2B	-2.74	1.31	1.37
2	g	200	HEM	CMB-C2B	2.73	1.56	1.50
2	v	200	HEM	FE-NA	2.71	2.04	1.95
2	L	200	HEM	CHA-C4D	2.70	1.43	1.38
2	C	200	HEM	CAC-C3C	2.70	1.54	1.47
2	g	200	HEM	CAB-C3B	2.69	1.54	1.47
2	P	200	HEM	C3C-C2C	-2.69	1.31	1.37
2	n	200	HEM	FE-ND	2.68	2.03	1.94
2	e	200	HEM	CAC-C3C	2.68	1.54	1.47
2	n	200	HEM	CHD-C1D	-2.67	1.33	1.39
2	F	200	HEM	C3C-C2C	-2.66	1.31	1.37
2	j	200	HEM	FE-NB	2.64	2.03	1.94
2	e	200	HEM	C3B-C2B	-2.64	1.31	1.37
2	F	200	HEM	C4A-NA	-2.64	1.34	1.39
2	k	200	HEM	C4A-NA	-2.63	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	200	HEM	C3C-C2C	-2.62	1.31	1.37
2	g	200	HEM	C4A-NA	-2.62	1.34	1.39
2	j	200	HEM	C1C-C2C	-2.61	1.40	1.45
2	t	200	HEM	CHA-C1A	-2.61	1.33	1.39
2	v	200	HEM	CHD-C1D	-2.61	1.33	1.39
2	S	200	HEM	FE-NA	-2.61	1.86	1.95
2	k	200	HEM	O2D-CGD	-2.58	1.22	1.30
2	F	200	HEM	CMC-C2C	2.58	1.56	1.50
2	B	200	HEM	CMC-C2C	2.57	1.56	1.50
2	C	200	HEM	C2A-C3A	-2.57	1.32	1.38
2	c	200	HEM	CAC-C3C	2.57	1.54	1.47
2	n	200	HEM	CAB-C3B	2.55	1.54	1.47
2	C	200	HEM	C4B-NB	2.54	1.43	1.38
2	M	200	HEM	CMD-C2D	2.53	1.56	1.50
2	j	200	HEM	C1A-C2A	-2.53	1.39	1.44
2	q	200	HEM	C2A-C3A	-2.52	1.32	1.38
2	g	200	HEM	C1C-NC	-2.52	1.34	1.39
2	C	200	HEM	CMB-C2B	2.52	1.55	1.50
2	g	200	HEM	FE-ND	2.52	2.02	1.94
2	R	200	HEM	C1D-ND	-2.51	1.33	1.38
2	M	200	HEM	C1B-NB	-2.51	1.35	1.40
2	S	200	HEM	CMA-C3A	2.51	1.55	1.50
2	c	200	HEM	CAB-C3B	2.50	1.54	1.47
2	c	200	HEM	FE-NC	2.48	2.03	1.95
2	S	200	HEM	C3C-C4C	2.48	1.50	1.46
2	q	200	HEM	C1C-NC	-2.48	1.34	1.39
2	F	200	HEM	C2A-C3A	-2.47	1.32	1.38
2	I	200	HEM	CAB-C3B	2.47	1.54	1.47
2	H	200	HEM	C2A-C3A	-2.47	1.32	1.38
2	U	200	HEM	C2A-C3A	-2.47	1.32	1.38
2	M	200	HEM	CAD-C3D	2.46	1.57	1.51
2	I	200	HEM	FE-NC	-2.46	1.87	1.95
2	o	200	HEM	CAB-C3B	2.45	1.53	1.47
2	C	200	HEM	C4A-C3A	-2.45	1.37	1.43
2	g	200	HEM	CAD-C3D	2.44	1.57	1.51
2	U	200	HEM	O2A-CGA	-2.44	1.22	1.30
2	R	200	HEM	C2A-C3A	-2.43	1.32	1.38
2	R	200	HEM	C3C-C2C	-2.43	1.32	1.37
2	F	200	HEM	CAB-C3B	2.42	1.53	1.47
2	U	200	HEM	C4C-NC	-2.41	1.35	1.39
2	j	200	HEM	CAD-C3D	2.41	1.57	1.51
2	R	200	HEM	CAB-C3B	2.39	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	j	200	HEM	CMB-C2B	2.39	1.55	1.50
2	B	200	HEM	CMB-C2B	2.39	1.55	1.50
2	I	200	HEM	CHA-C4D	-2.39	1.33	1.38
2	q	200	HEM	C4A-NA	-2.36	1.35	1.39
2	q	200	HEM	C3B-C2B	-2.36	1.32	1.37
2	k	200	HEM	FE-ND	2.36	2.02	1.94
2	I	200	HEM	C3B-C2B	-2.35	1.32	1.37
2	M	200	HEM	CMA-C3A	2.35	1.55	1.50
2	P	200	HEM	CMB-C2B	2.35	1.55	1.50
2	x	200	HEM	C1B-NB	-2.33	1.36	1.40
2	t	200	HEM	O2D-CGD	-2.32	1.23	1.30
2	j	200	HEM	C2A-C3A	-2.32	1.32	1.38
2	o	200	HEM	C3B-C2B	-2.31	1.32	1.37
2	S	200	HEM	C1D-ND	-2.31	1.34	1.38
2	I	200	HEM	C4B-NB	-2.30	1.34	1.38
2	M	200	HEM	C2A-C3A	-2.29	1.32	1.38
2	L	200	HEM	C1A-C2A	2.29	1.49	1.44
2	q	200	HEM	CAB-C3B	2.28	1.53	1.47
2	j	200	HEM	O1D-CGD	2.28	1.29	1.22
2	a	200	HEM	CMD-C2D	2.27	1.55	1.50
2	q	200	HEM	O2D-CGD	-2.25	1.23	1.30
2	P	200	HEM	FE-NB	2.24	2.01	1.94
2	j	200	HEM	CAC-C3C	2.24	1.53	1.47
2	x	200	HEM	C2A-C3A	-2.24	1.33	1.38
2	B	200	HEM	C4D-C3D	-2.23	1.41	1.45
2	R	200	HEM	C4C-NC	-2.23	1.35	1.39
2	L	200	HEM	C1D-ND	2.23	1.43	1.38
2	S	200	HEM	CHD-C1D	-2.23	1.34	1.39
2	R	200	HEM	C3B-C2B	-2.23	1.32	1.37
2	U	200	HEM	CAB-C3B	2.23	1.53	1.47
2	R	200	HEM	CMC-C2C	2.22	1.55	1.50
2	F	200	HEM	O2A-CGA	-2.22	1.23	1.30
2	I	200	HEM	CMB-C2B	2.22	1.55	1.50
2	X	200	HEM	CHA-C1A	2.22	1.44	1.39
2	k	200	HEM	CAB-C3B	2.22	1.53	1.47
2	C	200	HEM	CMA-C3A	2.21	1.55	1.50
2	M	200	HEM	C3C-C2C	-2.21	1.32	1.37
2	B	200	HEM	CAC-C3C	2.20	1.53	1.47
2	R	200	HEM	O2A-CGA	-2.20	1.23	1.30
2	M	200	HEM	CAB-C3B	2.20	1.53	1.47
2	n	200	HEM	C4A-NA	-2.19	1.35	1.39
2	e	200	HEM	CAD-C3D	2.19	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	200	HEM	CAA-C2A	2.19	1.57	1.51
2	n	200	HEM	CAA-C2A	2.18	1.56	1.51
2	t	200	HEM	C1B-NB	-2.17	1.36	1.40
2	o	200	HEM	C4A-NA	-2.17	1.35	1.39
2	g	200	HEM	CAA-C2A	2.17	1.56	1.51
2	B	200	HEM	O1A-CGA	2.17	1.29	1.22
2	C	200	HEM	C4D-ND	2.15	1.43	1.40
2	g	200	HEM	C3B-C2B	-2.14	1.32	1.37
2	a	200	HEM	CAC-C3C	2.14	1.53	1.47
2	x	200	HEM	CHC-C1C	-2.14	1.34	1.38
2	I	200	HEM	C1A-NA	2.14	1.43	1.39
2	k	200	HEM	CHB-C1B	-2.13	1.34	1.38
2	x	200	HEM	FE-NC	2.13	2.02	1.95
2	a	200	HEM	CMB-C2B	2.12	1.55	1.50
2	o	200	HEM	O2D-CGD	-2.12	1.23	1.30
2	C	200	HEM	CMD-C2D	2.11	1.55	1.50
2	q	200	HEM	O2A-CGA	-2.11	1.23	1.30
2	e	200	HEM	CAA-C2A	2.11	1.56	1.51
2	o	200	HEM	CHB-C1B	-2.10	1.34	1.38
2	v	200	HEM	CHB-C4A	-2.09	1.34	1.39
2	x	200	HEM	CMC-C2C	2.09	1.55	1.50
2	g	200	HEM	CAC-C3C	2.09	1.53	1.47
2	C	200	HEM	CHB-C1B	-2.09	1.34	1.38
2	o	200	HEM	CAC-C3C	2.09	1.53	1.47
2	L	200	HEM	CHB-C1B	-2.09	1.34	1.38
2	x	200	HEM	O2D-CGD	-2.08	1.23	1.30
2	S	200	HEM	C2A-C3A	-2.08	1.33	1.38
2	L	200	HEM	C1B-NB	-2.08	1.36	1.40
2	k	200	HEM	CAD-C3D	2.08	1.56	1.51
2	v	200	HEM	O2D-CGD	-2.07	1.24	1.30
2	a	200	HEM	CAD-C3D	2.07	1.56	1.51
2	X	200	HEM	C3C-C4C	-2.07	1.42	1.46
2	P	200	HEM	FE-NC	2.07	2.02	1.95
2	I	200	HEM	O1D-CGD	2.06	1.28	1.22
2	M	200	HEM	CAA-C2A	2.05	1.56	1.51
2	S	200	HEM	C1D-C2D	-2.05	1.40	1.44
2	n	200	HEM	C4C-NC	-2.05	1.35	1.39
2	H	200	HEM	CAB-C3B	2.04	1.52	1.47
2	X	200	HEM	CAD-C3D	2.04	1.56	1.51
2	U	200	HEM	O2D-CGD	-2.04	1.24	1.30
2	H	200	HEM	O1A-CGA	2.02	1.28	1.22
2	a	200	HEM	O1D-CGD	2.02	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	k	200	HEM	CMC-C2C	2.02	1.54	1.50
2	t	200	HEM	CAB-C3B	2.01	1.52	1.47
2	k	200	HEM	C1A-NA	-2.01	1.35	1.39
2	P	200	HEM	CMD-C2D	2.01	1.54	1.50
2	c	200	HEM	CMA-C3A	2.01	1.54	1.50
2	X	200	HEM	O2D-CGD	-2.01	1.24	1.30
2	S	200	HEM	CBD-CGD	2.00	1.55	1.50

All (439) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	200	HEM	CHD-C1D-ND	16.12	141.77	124.42
2	C	200	HEM	CHD-C4C-NC	-11.97	111.42	124.45
2	C	200	HEM	CHD-C1D-C2D	-9.92	109.36	125.03
2	S	200	HEM	C3D-C4D-ND	7.55	118.45	110.17
2	R	200	HEM	C4D-ND-C1D	7.44	114.01	105.21
2	x	200	HEM	C4D-ND-C1D	7.32	113.88	105.21
2	L	200	HEM	C4D-ND-C1D	7.11	113.63	105.21
2	F	200	HEM	C4D-ND-C1D	6.77	113.22	105.21
2	c	200	HEM	C4D-ND-C1D	6.61	113.03	105.21
2	X	200	HEM	C3B-C4B-NB	-6.54	104.77	109.47
2	j	200	HEM	C3B-C4B-NB	-6.52	104.79	109.47
2	a	200	HEM	C4C-C3C-C2C	6.48	112.44	106.81
2	H	200	HEM	C4D-ND-C1D	6.43	112.83	105.21
2	j	200	HEM	CHD-C4C-NC	-6.42	117.46	124.45
2	a	200	HEM	C4D-ND-C1D	6.35	112.73	105.21
2	o	200	HEM	C4D-ND-C1D	6.33	112.70	105.21
2	X	200	HEM	C4D-ND-C1D	6.26	112.62	105.21
2	S	200	HEM	CAD-C3D-C4D	6.23	135.55	124.70
2	C	200	HEM	CHB-C4A-NA	6.22	135.13	123.86
2	C	200	HEM	CHD-C4C-C3C	6.16	135.60	125.21
2	X	200	HEM	C1B-NB-C4B	6.10	112.43	105.21
2	j	200	HEM	C4D-ND-C1D	6.00	112.32	105.21
2	L	200	HEM	CHC-C1C-NC	5.91	130.89	124.45
2	U	200	HEM	C4D-ND-C1D	5.88	112.17	105.21
2	I	200	HEM	C4D-ND-C1D	5.83	112.11	105.21
2	j	200	HEM	CHC-C4B-NB	5.80	130.66	124.42
2	S	200	HEM	C4D-C3D-C2D	-5.80	98.45	106.89
2	S	200	HEM	C4A-CHB-C1B	-5.60	113.08	126.25
2	v	200	HEM	C3B-C4B-NB	-5.54	105.49	109.47
2	o	200	HEM	CMD-C2D-C1D	5.52	133.65	125.03
2	j	200	HEM	C1B-NB-C4B	5.38	111.58	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	200	HEM	CBA-CAA-C2A	-5.38	97.67	112.53
2	X	200	HEM	C2A-C1A-NA	-5.36	104.20	110.15
2	a	200	HEM	CAA-CBA-CGA	-5.36	99.45	113.67
2	C	200	HEM	CHB-C4A-C3A	-5.18	112.39	127.43
2	e	200	HEM	C3B-C4B-NB	-5.06	105.83	109.47
2	H	200	HEM	C3B-C4B-NB	-5.03	105.86	109.47
2	U	200	HEM	C3B-C4B-NB	-5.00	105.88	109.47
2	L	200	HEM	C2A-C1A-NA	-4.97	104.63	110.15
2	P	200	HEM	CBD-CAD-C3D	-4.94	98.89	112.53
2	j	200	HEM	C4C-NC-C1C	-4.91	97.81	105.82
2	j	200	HEM	CBD-CAD-C3D	-4.91	98.96	112.53
2	v	200	HEM	C4D-ND-C1D	4.90	111.01	105.21
2	U	200	HEM	C1B-NB-C4B	4.88	110.99	105.21
2	e	200	HEM	CHD-C1D-ND	4.82	129.61	124.42
2	x	200	HEM	CHC-C4B-NB	4.74	129.52	124.42
2	F	200	HEM	C3B-C4B-NB	-4.72	106.08	109.47
2	U	200	HEM	C4C-C3C-C2C	4.70	110.89	106.81
2	k	200	HEM	C4D-ND-C1D	4.69	110.76	105.21
2	U	200	HEM	C3B-C2B-C1B	4.65	109.90	106.41
2	j	200	HEM	CAA-CBA-CGA	-4.65	101.34	113.67
2	a	200	HEM	CBD-CAD-C3D	-4.59	99.85	112.53
2	S	200	HEM	C4D-ND-C1D	-4.57	99.80	105.21
2	S	200	HEM	CBD-CAD-C3D	-4.56	99.92	112.53
2	n	200	HEM	C4D-ND-C1D	4.54	110.58	105.21
2	a	200	HEM	C2A-C1A-NA	-4.52	105.14	110.15
2	v	200	HEM	CHC-C1C-NC	4.52	129.37	124.45
2	e	200	HEM	C4D-ND-C1D	4.46	110.48	105.21
2	C	200	HEM	CHC-C1C-NC	4.45	129.30	124.45
2	C	200	HEM	CHA-C1A-C2A	4.45	135.04	125.30
2	c	200	HEM	C4C-C3C-C2C	4.43	110.65	106.81
2	I	200	HEM	C4A-NA-C1A	-4.40	98.65	105.82
2	v	200	HEM	CHD-C4C-NC	4.38	129.22	124.45
2	X	200	HEM	C4A-NA-C1A	4.38	112.96	105.82
2	j	200	HEM	C2C-C1C-NC	4.37	117.72	109.64
2	H	200	HEM	CBD-CAD-C3D	-4.33	100.57	112.53
2	c	200	HEM	CBA-CAA-C2A	-4.31	100.63	112.53
2	S	200	HEM	CHA-C4D-ND	-4.28	119.07	124.37
2	C	200	HEM	C4D-ND-C1D	4.27	110.27	105.21
2	I	200	HEM	CAA-CBA-CGA	4.26	124.97	113.67
2	H	200	HEM	C1B-NB-C4B	4.25	110.24	105.21
2	t	200	HEM	C3D-C4D-ND	4.25	114.83	110.17
2	L	200	HEM	CHB-C1B-NB	-4.22	119.15	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	q	200	HEM	C4D-ND-C1D	4.21	110.19	105.21
2	c	200	HEM	CHC-C1C-NC	4.20	129.03	124.45
2	g	200	HEM	CBD-CAD-C3D	4.18	124.10	112.53
2	R	200	HEM	C3B-C4B-NB	-4.18	106.47	109.47
2	a	200	HEM	CBC-CAC-C3C	-4.14	106.86	127.53
2	a	200	HEM	C4C-NC-C1C	4.09	112.49	105.82
2	x	200	HEM	C4A-NA-C1A	4.07	112.45	105.82
2	S	200	HEM	C2D-C1D-ND	4.06	114.59	109.90
2	I	200	HEM	C1B-NB-C4B	4.05	110.00	105.21
2	F	200	HEM	C4C-C3C-C2C	4.01	110.29	106.81
2	S	200	HEM	CHD-C1D-ND	-4.01	120.11	124.42
2	C	200	HEM	CMA-C3A-C4A	-3.98	119.36	125.42
2	U	200	HEM	CBA-CAA-C2A	-3.97	101.55	112.53
2	P	200	HEM	CHC-C1C-NC	3.97	128.77	124.45
2	L	200	HEM	CAD-CBD-CGD	-3.95	103.19	113.67
2	e	200	HEM	C1B-NB-C4B	3.94	109.88	105.21
2	k	200	HEM	C4C-C3C-C2C	3.94	110.23	106.81
2	L	200	HEM	CBA-CAA-C2A	-3.91	101.72	112.53
2	e	200	HEM	CHB-C1B-NB	3.91	129.20	124.37
2	H	200	HEM	CHC-C1C-NC	3.89	128.69	124.45
2	C	200	HEM	CHB-C1B-NB	-3.88	119.56	124.37
2	M	200	HEM	CAD-C3D-C4D	3.87	131.45	124.70
2	t	200	HEM	CMB-C2B-C1B	3.85	131.04	125.03
2	H	200	HEM	CBA-CAA-C2A	-3.84	101.93	112.53
2	v	200	HEM	CHC-C4B-C3B	3.83	132.72	125.07
2	o	200	HEM	CHA-C4D-ND	3.81	129.08	124.37
2	j	200	HEM	C3C-C2C-C1C	-3.78	103.47	107.05
2	P	200	HEM	C2D-C1D-ND	3.77	114.26	109.90
2	X	200	HEM	CHA-C1A-C2A	3.77	133.54	125.30
2	R	200	HEM	C1B-NB-C4B	3.76	109.67	105.21
2	j	200	HEM	CHD-C1D-ND	3.76	128.47	124.42
2	I	200	HEM	CBD-CAD-C3D	-3.76	102.14	112.53
2	L	200	HEM	C3D-C4D-ND	-3.74	106.07	110.17
2	v	200	HEM	CAB-C3B-C2B	-3.73	116.30	128.43
2	R	200	HEM	C2A-C1A-NA	-3.73	106.01	110.15
2	C	200	HEM	CMA-C3A-C2A	3.72	133.50	125.62
2	M	200	HEM	C4D-ND-C1D	3.71	109.59	105.21
2	C	200	HEM	CAD-C3D-C4D	3.69	131.13	124.70
2	U	200	HEM	C2B-C1B-NB	-3.69	105.60	109.84
2	j	200	HEM	C3B-C2B-C1B	3.67	109.17	106.41
2	x	200	HEM	CBA-CAA-C2A	-3.65	102.44	112.53
2	v	200	HEM	CAA-C2A-C1A	3.65	132.06	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	o	200	HEM	CAC-C3C-C4C	3.64	133.52	124.82
2	g	200	HEM	CHD-C4C-C3C	3.63	131.33	125.21
2	S	200	HEM	CHC-C4B-NB	3.63	128.32	124.42
2	X	200	HEM	CMB-C2B-C1B	3.62	130.69	125.03
2	S	200	HEM	CMB-C2B-C1B	-3.61	119.39	125.03
2	x	200	HEM	CAA-CBA-CGA	3.59	123.19	113.67
2	P	200	HEM	C1D-C2D-C3D	-3.58	103.22	106.98
2	x	200	HEM	C3A-C4A-NA	-3.57	104.42	110.14
2	M	200	HEM	CAA-C2A-C1A	3.57	131.91	124.94
2	a	200	HEM	CMB-C2B-C1B	-3.55	119.49	125.03
2	j	200	HEM	CHC-C1C-C2C	-3.54	118.13	125.49
2	I	200	HEM	C3C-C2C-C1C	3.53	110.39	107.05
2	X	200	HEM	CHA-C4D-ND	3.51	128.71	124.37
2	I	200	HEM	CHC-C1C-NC	3.50	128.26	124.45
2	C	200	HEM	CMD-C2D-C1D	-3.49	119.57	125.03
2	L	200	HEM	CHD-C1D-ND	3.47	128.16	124.42
2	j	200	HEM	C2B-C1B-NB	-3.47	105.85	109.84
2	M	200	HEM	CAD-CBD-CGD	-3.47	104.46	113.67
2	g	200	HEM	C4C-NC-C1C	3.47	111.47	105.82
2	F	200	HEM	CAD-C3D-C4D	3.45	130.71	124.70
2	P	200	HEM	CHD-C1D-C2D	-3.45	119.58	125.03
2	I	200	HEM	C4D-C3D-C2D	-3.45	101.88	106.89
2	C	200	HEM	CAD-C3D-C2D	-3.44	121.42	127.87
2	U	200	HEM	CAA-CBA-CGA	3.42	122.74	113.67
2	a	200	HEM	C4A-NA-C1A	3.42	111.39	105.82
2	H	200	HEM	C4C-NC-C1C	3.41	111.38	105.82
2	M	200	HEM	C1B-NB-C4B	3.40	109.24	105.21
2	X	200	HEM	C3A-C4A-NA	-3.40	104.69	110.14
2	v	200	HEM	CHA-C4D-ND	3.39	128.56	124.37
2	c	200	HEM	CAD-C3D-C4D	3.39	130.61	124.70
2	j	200	HEM	CHB-C1B-NB	3.39	128.56	124.37
2	g	200	HEM	CHD-C1D-ND	3.39	128.07	124.42
2	C	200	HEM	C3D-C4D-ND	-3.37	106.47	110.17
2	k	200	HEM	CHB-C1B-NB	3.37	128.54	124.37
2	P	200	HEM	CMD-C2D-C3D	3.37	135.27	126.15
2	M	200	HEM	C3B-C2B-C1B	3.37	108.94	106.41
2	c	200	HEM	CMD-C2D-C1D	3.36	130.29	125.03
2	R	200	HEM	C4A-NA-C1A	3.36	111.30	105.82
2	n	200	HEM	CMD-C2D-C1D	3.36	130.28	125.03
2	v	200	HEM	O1D-CGD-CBD	-3.35	112.45	123.09
2	q	200	HEM	CHC-C4B-NB	3.35	128.03	124.42
2	x	200	HEM	C4C-C3C-C2C	3.34	109.71	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	x	200	HEM	C1B-NB-C4B	3.34	109.16	105.21
2	j	200	HEM	C2D-C1D-ND	-3.33	106.06	109.90
2	C	200	HEM	C2A-C1A-NA	-3.32	106.47	110.15
2	B	200	HEM	C4C-C3C-C2C	3.30	109.68	106.81
2	x	200	HEM	C2A-C1A-NA	-3.29	106.51	110.15
2	e	200	HEM	C3B-C2B-C1B	3.28	108.88	106.41
2	L	200	HEM	CHD-C4C-C3C	3.28	130.74	125.21
2	g	200	HEM	CHC-C4B-NB	3.27	127.94	124.42
2	v	200	HEM	C1D-C2D-C3D	-3.26	103.55	106.98
2	c	200	HEM	CHD-C4C-C3C	3.25	130.69	125.21
2	a	200	HEM	CHD-C4C-NC	3.23	127.97	124.45
2	q	200	HEM	CHD-C4C-C3C	3.23	130.65	125.21
2	x	200	HEM	C3B-C4B-NB	-3.22	107.15	109.47
2	j	200	HEM	CHD-C4C-C3C	3.22	130.64	125.21
2	L	200	HEM	C4C-NC-C1C	3.22	111.07	105.82
2	t	200	HEM	CHA-C4D-C3D	-3.21	119.31	125.23
2	a	200	HEM	CHD-C1D-C2D	3.20	130.08	125.03
2	e	200	HEM	CMD-C2D-C1D	-3.18	120.06	125.03
2	I	200	HEM	C3A-C4A-NA	3.17	115.23	110.14
2	v	200	HEM	O2D-CGD-O1D	3.15	131.42	123.33
2	a	200	HEM	CHD-C1D-ND	-3.14	121.04	124.42
2	L	200	HEM	C4A-NA-C1A	3.14	110.94	105.82
2	o	200	HEM	CAC-C3C-C2C	-3.13	118.25	128.43
2	F	200	HEM	C1B-NB-C4B	3.13	108.91	105.21
2	L	200	HEM	CAD-C3D-C4D	3.10	130.10	124.70
2	t	200	HEM	C4D-C3D-C2D	-3.10	102.38	106.89
2	U	200	HEM	C4C-NC-C1C	3.10	110.87	105.82
2	L	200	HEM	CMA-C3A-C2A	3.06	132.12	125.62
2	a	200	HEM	C3B-C4B-NB	-3.06	107.27	109.47
2	t	200	HEM	CHD-C4C-C3C	3.05	130.35	125.21
2	c	200	HEM	C4B-C3B-C2B	3.04	110.08	107.28
2	c	200	HEM	CMA-C3A-C2A	3.04	132.07	125.62
2	a	200	HEM	C3C-C2C-C1C	-3.03	104.18	107.05
2	M	200	HEM	CMA-C3A-C4A	3.02	130.01	125.42
2	H	200	HEM	C2A-C1A-NA	-3.01	106.81	110.15
2	B	200	HEM	CAD-CBD-CGD	-3.01	105.68	113.67
2	H	200	HEM	C2B-C1B-NB	-2.98	106.41	109.84
2	C	200	HEM	CHA-C1A-NA	-2.98	118.45	123.86
2	X	200	HEM	C2B-C1B-NB	-2.98	106.41	109.84
2	B	200	HEM	C1D-C2D-C3D	-2.98	103.85	106.98
2	j	200	HEM	CBC-CAC-C3C	-2.97	112.68	127.53
2	v	200	HEM	C1B-NB-C4B	2.97	108.72	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	200	HEM	O1A-CGA-CBA	-2.96	113.69	123.09
2	v	200	HEM	O2A-CGA-CBA	2.95	123.33	114.00
2	x	200	HEM	C4A-C3A-C2A	2.95	110.19	106.82
2	v	200	HEM	O1A-CGA-CBA	-2.95	113.75	123.09
2	k	200	HEM	CBB-CAB-C3B	-2.94	112.82	127.53
2	X	200	HEM	CHC-C4B-NB	2.93	127.58	124.42
2	o	200	HEM	CHD-C4C-C3C	2.93	130.15	125.21
2	X	200	HEM	C4C-C3C-C2C	2.92	109.35	106.81
2	x	200	HEM	C4B-C3B-C2B	2.92	109.97	107.28
2	S	200	HEM	CMA-C3A-C4A	-2.92	120.97	125.42
2	F	200	HEM	CHC-C4B-NB	2.91	127.56	124.42
2	e	200	HEM	C4A-C3A-C2A	2.91	110.15	106.82
2	t	200	HEM	CMD-C2D-C1D	2.91	129.58	125.03
2	v	200	HEM	C4A-C3A-C2A	2.90	110.14	106.82
2	I	200	HEM	CHD-C1D-ND	2.90	127.55	124.42
2	S	200	HEM	CAA-C2A-C1A	2.89	130.59	124.94
2	L	200	HEM	CAD-C3D-C2D	-2.89	122.45	127.87
2	X	200	HEM	CBC-CAC-C3C	-2.89	113.08	127.53
2	S	200	HEM	CHD-C4C-NC	-2.89	121.31	124.45
2	t	200	HEM	CMB-C2B-C3B	-2.89	121.44	128.43
2	I	200	HEM	O2A-CGA-CBA	2.88	123.11	114.00
2	c	200	HEM	CAD-CBD-CGD	-2.87	106.06	113.67
2	e	200	HEM	C2B-C1B-NB	-2.86	106.56	109.84
2	F	200	HEM	C1A-CHA-C4D	2.85	132.95	126.25
2	x	200	HEM	C2B-C1B-NB	-2.85	106.57	109.84
2	R	200	HEM	C1A-CHA-C4D	2.85	132.94	126.25
2	I	200	HEM	O1A-CGA-CBA	-2.83	114.10	123.09
2	M	200	HEM	CHC-C1C-NC	2.83	127.54	124.45
2	B	200	HEM	C2A-C1A-NA	-2.83	107.01	110.15
2	L	200	HEM	C2D-C1D-ND	-2.82	106.65	109.90
2	I	200	HEM	C3B-C4B-NB	-2.81	107.45	109.47
2	q	200	HEM	C2A-C1A-NA	-2.81	107.03	110.15
2	B	200	HEM	C4C-NC-C1C	2.81	110.40	105.82
2	S	200	HEM	CHD-C4C-C3C	2.81	129.94	125.21
2	H	200	HEM	C4C-C3C-C2C	2.80	109.24	106.81
2	L	200	HEM	C3C-C2C-C1C	2.80	109.69	107.05
2	v	200	HEM	C4C-C3C-C2C	2.79	109.24	106.81
2	n	200	HEM	CMC-C2C-C1C	2.78	129.62	124.73
2	C	200	HEM	CMD-C2D-C3D	2.78	133.66	126.15
2	I	200	HEM	CHD-C4C-NC	-2.77	121.43	124.45
2	v	200	HEM	CBD-CAD-C3D	-2.77	104.88	112.53
2	X	200	HEM	CHD-C4C-NC	2.76	127.45	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	x	200	HEM	CHA-C4D-ND	2.76	127.78	124.37
2	g	200	HEM	CBC-CAC-C3C	-2.75	113.78	127.53
2	x	200	HEM	CMB-C2B-C1B	2.75	129.32	125.03
2	c	200	HEM	C2A-C1A-NA	-2.74	107.11	110.15
2	M	200	HEM	CHC-C4B-NB	-2.74	121.47	124.42
2	n	200	HEM	O2D-CGD-CBD	2.74	122.66	114.00
2	n	200	HEM	C1D-C2D-C3D	-2.74	104.10	106.98
2	j	200	HEM	C4A-C3A-C2A	2.74	109.95	106.82
2	F	200	HEM	C4C-NC-C1C	2.74	110.28	105.82
2	t	200	HEM	CAA-CBA-CGA	-2.74	106.41	113.67
2	t	200	HEM	CBD-CAD-C3D	2.73	120.09	112.53
2	X	200	HEM	C2D-C1D-ND	-2.73	106.75	109.90
2	P	200	HEM	CBC-CAC-C3C	-2.72	113.91	127.53
2	L	200	HEM	C1C-CHC-C4B	2.71	131.78	126.02
2	e	200	HEM	CMD-C2D-C3D	2.71	133.48	126.15
2	X	200	HEM	O2A-CGA-CBA	2.71	122.57	114.00
2	v	200	HEM	C3B-C2B-C1B	2.69	108.43	106.41
2	L	200	HEM	CMD-C2D-C1D	2.68	129.22	125.03
2	g	200	HEM	C2A-C1A-NA	-2.67	107.19	110.15
2	j	200	HEM	C4C-C3C-C2C	2.67	109.13	106.81
2	a	200	HEM	CMA-C3A-C4A	-2.67	121.36	125.42
2	n	200	HEM	CMC-C2C-C3C	-2.66	121.98	128.43
2	c	200	HEM	C2D-C1D-ND	-2.66	106.83	109.90
2	U	200	HEM	CMC-C2C-C1C	2.65	129.40	124.73
2	L	200	HEM	CMA-C3A-C4A	-2.65	121.38	125.42
2	L	200	HEM	CHB-C4A-NA	2.64	128.64	123.86
2	H	200	HEM	CBB-CAB-C3B	-2.63	114.36	127.53
2	P	200	HEM	O1A-CGA-CBA	-2.63	114.74	123.09
2	k	200	HEM	CAB-C3B-C2B	-2.63	119.88	128.43
2	S	200	HEM	CAC-C3C-C4C	2.62	131.07	124.82
2	I	200	HEM	CMD-C2D-C1D	-2.61	120.95	125.03
2	I	200	HEM	CHC-C4B-C3B	2.61	130.28	125.07
2	c	200	HEM	CMA-C3A-C4A	-2.61	121.45	125.42
2	X	200	HEM	CMD-C2D-C1D	2.61	129.11	125.03
2	v	200	HEM	CMD-C2D-C1D	2.60	129.10	125.03
2	g	200	HEM	O1D-CGD-CBD	-2.59	114.87	123.09
2	U	200	HEM	CBD-CAD-C3D	-2.59	105.38	112.53
2	S	200	HEM	CMD-C2D-C1D	-2.58	121.00	125.03
2	I	200	HEM	O1D-CGD-CBD	-2.58	114.90	123.09
2	e	200	HEM	CHC-C4B-NB	2.58	127.20	124.42
2	c	200	HEM	CAD-C3D-C2D	-2.57	123.06	127.87
2	U	200	HEM	CHD-C4C-NC	2.57	127.25	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	200	HEM	CBB-CAB-C3B	-2.56	114.73	127.53
2	B	200	HEM	CBC-CAC-C3C	-2.56	114.75	127.53
2	U	200	HEM	CMB-C2B-C3B	-2.55	122.25	128.43
2	c	200	HEM	C3D-C4D-ND	-2.55	107.38	110.17
2	k	200	HEM	CMC-C2C-C1C	2.52	129.17	124.73
2	R	200	HEM	C3A-C4A-NA	-2.52	106.10	110.14
2	n	200	HEM	C4C-C3C-C2C	2.52	109.00	106.81
2	k	200	HEM	C3B-C2B-C1B	2.51	108.30	106.41
2	a	200	HEM	O2A-CGA-O1A	2.51	129.80	123.33
2	q	200	HEM	C1D-C2D-C3D	-2.51	104.34	106.98
2	c	200	HEM	C4C-NC-C1C	2.51	109.92	105.82
2	B	200	HEM	CBD-CAD-C3D	-2.51	105.59	112.53
2	M	200	HEM	CAA-C2A-C3A	-2.51	121.44	127.07
2	S	200	HEM	CHA-C1A-NA	2.51	128.41	123.86
2	B	200	HEM	C4A-NA-C1A	2.51	109.91	105.82
2	c	200	HEM	CMB-C2B-C1B	2.51	128.95	125.03
2	g	200	HEM	C4D-C3D-C2D	-2.50	103.25	106.89
2	t	200	HEM	CMC-C2C-C1C	2.50	129.13	124.73
2	X	200	HEM	C4A-C3A-C2A	2.49	109.67	106.82
2	j	200	HEM	CMD-C2D-C1D	-2.49	121.14	125.03
2	X	200	HEM	CMB-C2B-C3B	-2.49	122.40	128.43
2	t	200	HEM	CBC-CAC-C3C	-2.48	115.14	127.53
2	v	200	HEM	C4C-CHD-C1D	-2.48	120.76	126.02
2	t	200	HEM	C2D-C1D-ND	2.47	112.76	109.90
2	g	200	HEM	C4A-NA-C1A	2.47	109.85	105.82
2	P	200	HEM	C4C-C3C-C2C	2.45	108.94	106.81
2	F	200	HEM	CAD-CBD-CGD	2.45	120.17	113.67
2	I	200	HEM	C2D-C1D-ND	-2.45	107.07	109.90
2	a	200	HEM	CHB-C1B-NB	2.45	127.40	124.37
2	n	200	HEM	C1A-CHA-C4D	2.45	132.00	126.25
2	X	200	HEM	CAA-CBA-CGA	-2.44	107.18	113.67
2	v	200	HEM	CHC-C4B-NB	-2.44	121.80	124.42
2	a	200	HEM	CMA-C3A-C2A	2.44	130.80	125.62
2	a	200	HEM	CMD-C2D-C1D	2.44	128.84	125.03
2	B	200	HEM	CHA-C4D-ND	2.44	127.38	124.37
2	C	200	HEM	CHC-C4B-NB	2.43	127.04	124.42
2	S	200	HEM	CMB-C2B-C3B	2.43	134.31	128.43
2	n	200	HEM	CBA-CAA-C2A	2.43	119.25	112.53
2	X	200	HEM	C4B-C3B-C2B	2.43	109.51	107.28
2	e	200	HEM	CHD-C4C-NC	-2.42	121.82	124.45
2	M	200	HEM	CMB-C2B-C1B	-2.42	121.25	125.03
2	L	200	HEM	CHD-C4C-NC	-2.41	121.83	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	200	HEM	C4C-NC-C1C	-2.40	101.91	105.82
2	U	200	HEM	C4A-C3A-C2A	2.40	109.56	106.82
2	M	200	HEM	O2A-CGA-CBA	2.40	121.58	114.00
2	v	200	HEM	CAB-C3B-C4B	2.40	134.98	124.39
2	e	200	HEM	CHD-C1D-C2D	-2.40	121.25	125.03
2	q	200	HEM	C4C-NC-C1C	2.39	109.72	105.82
2	H	200	HEM	O1D-CGD-CBD	-2.39	115.52	123.09
2	o	200	HEM	CHD-C1D-C2D	2.38	128.78	125.03
2	g	200	HEM	O2D-CGD-CBD	2.38	121.51	114.00
2	t	200	HEM	CAB-C3B-C2B	-2.37	120.71	128.43
2	B	200	HEM	C3B-C2B-C1B	2.37	108.19	106.41
2	t	200	HEM	CHD-C1D-C2D	-2.37	121.29	125.03
2	R	200	HEM	CAD-C3D-C4D	2.37	128.82	124.70
2	g	200	HEM	CHA-C1A-NA	2.37	128.15	123.86
2	L	200	HEM	C2C-C1C-NC	-2.37	105.26	109.64
2	H	200	HEM	CHB-C1B-NB	2.36	127.29	124.37
2	q	200	HEM	C4A-NA-C1A	2.36	109.67	105.82
2	I	200	HEM	CHC-C4B-NB	-2.34	121.90	124.42
2	P	200	HEM	C4A-CHB-C1B	-2.34	120.74	126.25
2	F	200	HEM	CMD-C2D-C1D	2.34	128.69	125.03
2	H	200	HEM	C3B-C2B-C1B	2.34	108.17	106.41
2	a	200	HEM	CHB-C4A-NA	2.34	128.10	123.86
2	g	200	HEM	CBB-CAB-C3B	-2.32	115.92	127.53
2	x	200	HEM	C1D-C2D-C3D	-2.32	104.54	106.98
2	c	200	HEM	CHA-C4D-ND	2.32	127.23	124.37
2	X	200	HEM	CHD-C1D-C2D	2.31	128.68	125.03
2	o	200	HEM	CMB-C2B-C1B	-2.31	121.43	125.03
2	g	200	HEM	C4A-C3A-C2A	2.31	109.46	106.82
2	R	200	HEM	CHD-C1D-C2D	2.30	128.66	125.03
2	U	200	HEM	CAC-C3C-C2C	-2.30	120.96	128.43
2	x	200	HEM	CBC-CAC-C3C	-2.30	116.05	127.53
2	a	200	HEM	CBB-CAB-C3B	-2.29	116.06	127.53
2	e	200	HEM	C4D-C3D-C2D	-2.29	103.55	106.89
2	M	200	HEM	CHC-C4B-C3B	2.28	129.63	125.07
2	o	200	HEM	C2D-C1D-ND	-2.28	107.27	109.90
2	v	200	HEM	CMC-C2C-C3C	-2.28	122.91	128.43
2	x	200	HEM	C3D-C4D-ND	-2.28	107.67	110.17
2	v	200	HEM	C3C-C2C-C1C	2.27	109.19	107.05
2	H	200	HEM	CAA-CBA-CGA	-2.27	107.64	113.67
2	P	200	HEM	CMD-C2D-C1D	-2.27	121.49	125.03
2	k	200	HEM	O2D-CGD-O1D	-2.26	117.51	123.33
2	a	200	HEM	CHD-C4C-C3C	2.25	129.01	125.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	200	HEM	CAB-C3B-C2B	-2.25	121.13	128.43
2	P	200	HEM	C3B-C2B-C1B	2.24	108.09	106.41
2	L	200	HEM	CHA-C1A-C2A	2.24	130.21	125.30
2	R	200	HEM	C4D-C3D-C2D	-2.24	103.63	106.89
2	H	200	HEM	O2D-CGD-CBD	2.24	121.08	114.00
2	C	200	HEM	CAA-C2A-C3A	-2.24	122.05	127.07
2	j	200	HEM	C4A-CHB-C1B	-2.24	120.98	126.25
2	S	200	HEM	O2A-CGA-CBA	2.23	121.04	114.00
2	M	200	HEM	CBD-CAD-C3D	2.23	118.69	112.53
2	P	200	HEM	C4C-CHD-C1D	-2.23	121.29	126.02
2	g	200	HEM	C4C-C3C-C2C	2.22	108.74	106.81
2	n	200	HEM	CAD-C3D-C4D	2.22	128.57	124.70
2	X	200	HEM	O2D-CGD-O1D	-2.21	117.64	123.33
2	F	200	HEM	C3B-C2B-C1B	2.21	108.07	106.41
2	j	200	HEM	CAC-C3C-C2C	-2.21	121.25	128.43
2	a	200	HEM	CMB-C2B-C3B	2.20	133.75	128.43
2	k	200	HEM	CBC-CAC-C3C	-2.20	116.53	127.53
2	o	200	HEM	CHC-C1C-NC	2.19	126.84	124.45
2	S	200	HEM	O2D-CGD-O1D	-2.19	117.71	123.33
2	j	200	HEM	C4A-NA-C1A	-2.18	102.27	105.82
2	S	200	HEM	CAC-C3C-C2C	-2.18	121.34	128.43
2	n	200	HEM	CAC-C3C-C2C	-2.18	121.35	128.43
2	x	200	HEM	CMC-C2C-C1C	2.18	128.56	124.73
2	L	200	HEM	O2A-CGA-CBA	2.17	120.86	114.00
2	X	200	HEM	CHB-C4A-NA	2.17	127.80	123.86
2	k	200	HEM	O2D-CGD-CBD	2.17	120.86	114.00
2	c	200	HEM	CBD-CAD-C3D	-2.17	106.54	112.53
2	k	200	HEM	C1A-CHA-C4D	2.16	131.33	126.25
2	U	200	HEM	CMD-C2D-C1D	2.16	128.41	125.03
2	c	200	HEM	CAA-C2A-C1A	-2.16	120.72	124.94
2	g	200	HEM	CHD-C1D-C2D	-2.16	121.62	125.03
2	H	200	HEM	C3D-C4D-ND	-2.15	107.81	110.17
2	S	200	HEM	C4B-C3B-C2B	2.15	109.25	107.28
2	R	200	HEM	C3D-C4D-ND	-2.14	107.82	110.17
2	v	200	HEM	C1A-C2A-C3A	-2.14	103.55	106.87
2	F	200	HEM	CAB-C3B-C2B	-2.14	121.48	128.43
2	F	200	HEM	C4B-C3B-C2B	2.13	109.24	107.28
2	P	200	HEM	CAD-C3D-C4D	2.12	128.40	124.70
2	C	200	HEM	C4A-CHB-C1B	-2.12	121.25	126.25
2	e	200	HEM	CBB-CAB-C3B	-2.12	116.94	127.53
2	k	200	HEM	C4D-C3D-C2D	-2.12	103.81	106.89
2	R	200	HEM	C4C-C3C-C2C	2.11	108.64	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	x	200	HEM	C2D-C1D-ND	-2.11	107.46	109.90
2	S	200	HEM	CMA-C3A-C2A	2.11	130.09	125.62
2	n	200	HEM	C1C-CHC-C4B	2.10	130.49	126.02
2	g	200	HEM	C4D-ND-C1D	2.10	107.70	105.21
2	S	200	HEM	O1A-CGA-CBA	-2.10	116.43	123.09
2	e	200	HEM	CAA-C2A-C1A	2.09	129.02	124.94
2	n	200	HEM	O2D-CGD-O1D	-2.09	117.97	123.33
2	g	200	HEM	CBA-CAA-C2A	-2.08	106.78	112.53
2	L	200	HEM	CAA-C2A-C1A	-2.08	120.88	124.94
2	v	200	HEM	C2C-C1C-NC	-2.08	105.80	109.64
2	U	200	HEM	CMC-C2C-C3C	-2.07	123.42	128.43
2	t	200	HEM	C4C-NC-C1C	2.07	109.19	105.82
2	k	200	HEM	C3B-C4B-NB	-2.06	107.98	109.47
2	e	200	HEM	CHD-C4C-C3C	2.06	128.69	125.21
2	v	200	HEM	C1A-CHA-C4D	2.05	131.06	126.25
2	j	200	HEM	CAD-C3D-C4D	2.04	128.26	124.70
2	M	200	HEM	C3C-C2C-C1C	2.04	108.98	107.05
2	t	200	HEM	CAD-C3D-C2D	2.04	131.69	127.87
2	P	200	HEM	CAA-C2A-C1A	2.04	128.93	124.94
2	v	200	HEM	CAD-CBD-CGD	2.04	119.07	113.67
2	M	200	HEM	C2B-C1B-NB	-2.04	107.50	109.84
2	x	200	HEM	CAA-C2A-C1A	2.04	128.91	124.94
2	a	200	HEM	C1A-CHA-C4D	2.03	131.03	126.25
2	k	200	HEM	CBD-CAD-C3D	2.03	118.15	112.53
2	t	200	HEM	CHD-C4C-NC	-2.03	122.24	124.45
2	x	200	HEM	CMB-C2B-C3B	-2.03	123.52	128.43
2	S	200	HEM	O2D-CGD-CBD	2.02	120.38	114.00
2	e	200	HEM	C1C-CHC-C4B	2.02	130.31	126.02
2	n	200	HEM	CAC-C3C-C4C	2.02	129.64	124.82
2	k	200	HEM	CHB-C1B-C2B	-2.00	121.26	126.95

There are no chirality outliers.

All (142) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	200	HEM	C3A-C2A-CAA-CBA
2	H	200	HEM	C2C-C3C-CAC-CBC
2	L	200	HEM	C3D-CAD-CBD-CGD
2	R	200	HEM	C1A-C2A-CAA-CBA
2	R	200	HEM	C2C-C3C-CAC-CBC
2	R	200	HEM	C4C-C3C-CAC-CBC
2	R	200	HEM	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
2	U	200	HEM	C2B-C3B-CAB-CBB
2	U	200	HEM	C4B-C3B-CAB-CBB
2	U	200	HEM	C2C-C3C-CAC-CBC
2	o	200	HEM	C2B-C3B-CAB-CBB
2	o	200	HEM	C4B-C3B-CAB-CBB
2	t	200	HEM	C2D-C3D-CAD-CBD
2	t	200	HEM	C4D-C3D-CAD-CBD
2	v	200	HEM	C2C-C3C-CAC-CBC
2	x	200	HEM	C2C-C3C-CAC-CBC
2	x	200	HEM	C4C-C3C-CAC-CBC
2	R	200	HEM	C2D-C3D-CAD-CBD
2	L	200	HEM	C4D-C3D-CAD-CBD
2	M	200	HEM	C4D-C3D-CAD-CBD
2	C	200	HEM	C1A-C2A-CAA-CBA
2	M	200	HEM	C2D-C3D-CAD-CBD
2	o	200	HEM	C2D-C3D-CAD-CBD
2	B	200	HEM	C2A-CAA-CBA-CGA
2	C	200	HEM	C2A-CAA-CBA-CGA
2	F	200	HEM	C3D-CAD-CBD-CGD
2	M	200	HEM	C3D-CAD-CBD-CGD
2	k	200	HEM	C3D-CAD-CBD-CGD
2	v	200	HEM	C2A-CAA-CBA-CGA
2	P	200	HEM	C1A-C2A-CAA-CBA
2	R	200	HEM	C3A-C2A-CAA-CBA
2	X	200	HEM	C2D-C3D-CAD-CBD
2	o	200	HEM	C4D-C3D-CAD-CBD
2	L	200	HEM	C2D-C3D-CAD-CBD
2	R	200	HEM	C3D-CAD-CBD-CGD
2	P	200	HEM	C3A-C2A-CAA-CBA
2	B	200	HEM	C4B-C3B-CAB-CBB
2	H	200	HEM	C4C-C3C-CAC-CBC
2	U	200	HEM	C4C-C3C-CAC-CBC
2	g	200	HEM	C4B-C3B-CAB-CBB
2	X	200	HEM	C4D-C3D-CAD-CBD
2	C	200	HEM	C3D-CAD-CBD-CGD
2	k	200	HEM	C2A-CAA-CBA-CGA
2	t	200	HEM	C2A-CAA-CBA-CGA
2	k	200	HEM	C4D-C3D-CAD-CBD
2	I	200	HEM	C2A-CAA-CBA-CGA
2	g	200	HEM	C2A-CAA-CBA-CGA
2	t	200	HEM	C3D-CAD-CBD-CGD
2	X	200	HEM	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
2	k	200	HEM	C2D-C3D-CAD-CBD
2	o	200	HEM	C1A-C2A-CAA-CBA
2	t	200	HEM	C1A-C2A-CAA-CBA
2	H	200	HEM	C4B-C3B-CAB-CBB
2	L	200	HEM	C4B-C3B-CAB-CBB
2	M	200	HEM	C4B-C3B-CAB-CBB
2	P	200	HEM	C4B-C3B-CAB-CBB
2	X	200	HEM	C4B-C3B-CAB-CBB
2	a	200	HEM	C4B-C3B-CAB-CBB
2	c	200	HEM	C4B-C3B-CAB-CBB
2	c	200	HEM	C4C-C3C-CAC-CBC
2	e	200	HEM	C4B-C3B-CAB-CBB
2	j	200	HEM	C4B-C3B-CAB-CBB
2	k	200	HEM	C4B-C3B-CAB-CBB
2	t	200	HEM	C4C-C3C-CAC-CBC
2	v	200	HEM	C4B-C3B-CAB-CBB
2	v	200	HEM	C4C-C3C-CAC-CBC
2	g	200	HEM	C3A-C2A-CAA-CBA
2	F	200	HEM	C4D-C3D-CAD-CBD
2	q	200	HEM	C4D-C3D-CAD-CBD
2	c	200	HEM	C2C-C3C-CAC-CBC
2	j	200	HEM	C3A-C2A-CAA-CBA
2	F	200	HEM	C4C-C3C-CAC-CBC
2	x	200	HEM	C4B-C3B-CAB-CBB
2	F	200	HEM	C2D-C3D-CAD-CBD
2	L	200	HEM	CAA-CBA-CGA-O2A
2	e	200	HEM	CAD-CBD-CGD-O1D
2	F	200	HEM	C2A-CAA-CBA-CGA
2	R	200	HEM	C2A-CAA-CBA-CGA
2	S	200	HEM	CAD-CBD-CGD-O2D
2	L	200	HEM	CAA-CBA-CGA-O1A
2	e	200	HEM	CAA-CBA-CGA-O1A
2	M	200	HEM	CAD-CBD-CGD-O1D
2	n	200	HEM	CAA-CBA-CGA-O1A
2	c	200	HEM	CAD-CBD-CGD-O1D
2	g	200	HEM	CAA-CBA-CGA-O2A
2	M	200	HEM	CAD-CBD-CGD-O2D
2	R	200	HEM	CAA-CBA-CGA-O2A
2	k	200	HEM	CAA-CBA-CGA-O2A
2	t	200	HEM	CAD-CBD-CGD-O1D
2	v	200	HEM	CAA-CBA-CGA-O1A
2	q	200	HEM	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
2	q	200	HEM	CAA-CBA-CGA-O1A
2	H	200	HEM	CAA-CBA-CGA-O1A
2	S	200	HEM	CAA-CBA-CGA-O2A
2	e	200	HEM	CAD-CBD-CGD-O2D
2	S	200	HEM	CAD-CBD-CGD-O1D
2	e	200	HEM	CAA-CBA-CGA-O2A
2	n	200	HEM	CAA-CBA-CGA-O2A
2	R	200	HEM	CAA-CBA-CGA-O1A
2	k	200	HEM	CAA-CBA-CGA-O1A
2	v	200	HEM	CAA-CBA-CGA-O2A
2	v	200	HEM	CAD-CBD-CGD-O2D
2	g	200	HEM	CAA-CBA-CGA-O1A
2	c	200	HEM	CAD-CBD-CGD-O2D
2	H	200	HEM	C2A-CAA-CBA-CGA
2	S	200	HEM	CAA-CBA-CGA-O1A
2	o	200	HEM	C3A-C2A-CAA-CBA
2	H	200	HEM	CAA-CBA-CGA-O2A
2	C	200	HEM	CAD-CBD-CGD-O2D
2	L	200	HEM	CAD-CBD-CGD-O1D
2	t	200	HEM	CAD-CBD-CGD-O2D
2	C	200	HEM	CAA-CBA-CGA-O2A
2	q	200	HEM	CAA-CBA-CGA-O2A
2	F	200	HEM	C2C-C3C-CAC-CBC
2	x	200	HEM	C2B-C3B-CAB-CBB
2	L	200	HEM	CAD-CBD-CGD-O2D
2	P	200	HEM	CAA-CBA-CGA-O2A
2	C	200	HEM	CAA-CBA-CGA-O1A
2	t	200	HEM	CAA-CBA-CGA-O1A
2	k	200	HEM	C4C-C3C-CAC-CBC
2	o	200	HEM	C4C-C3C-CAC-CBC
2	e	200	HEM	C3D-CAD-CBD-CGD
2	P	200	HEM	CAA-CBA-CGA-O1A
2	v	200	HEM	CAD-CBD-CGD-O1D
2	t	200	HEM	C3A-C2A-CAA-CBA
2	t	200	HEM	CAA-CBA-CGA-O2A
2	X	200	HEM	C3A-C2A-CAA-CBA
2	g	200	HEM	C1A-C2A-CAA-CBA
2	C	200	HEM	CAD-CBD-CGD-O1D
2	X	200	HEM	CAA-CBA-CGA-O1A
2	k	200	HEM	C3A-C2A-CAA-CBA
2	X	200	HEM	CAA-CBA-CGA-O2A
2	c	200	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
2	B	200	HEM	CAA-CBA-CGA-O2A
2	I	200	HEM	C2B-C3B-CAB-CBB
2	M	200	HEM	CAA-CBA-CGA-O2A
2	o	200	HEM	CAD-CBD-CGD-O1D
2	M	200	HEM	CAA-CBA-CGA-O1A
2	x	200	HEM	CAD-CBD-CGD-O2D
2	c	200	HEM	CAA-CBA-CGA-O2A
2	I	200	HEM	CAA-CBA-CGA-O2A
2	k	200	HEM	CAD-CBD-CGD-O2D

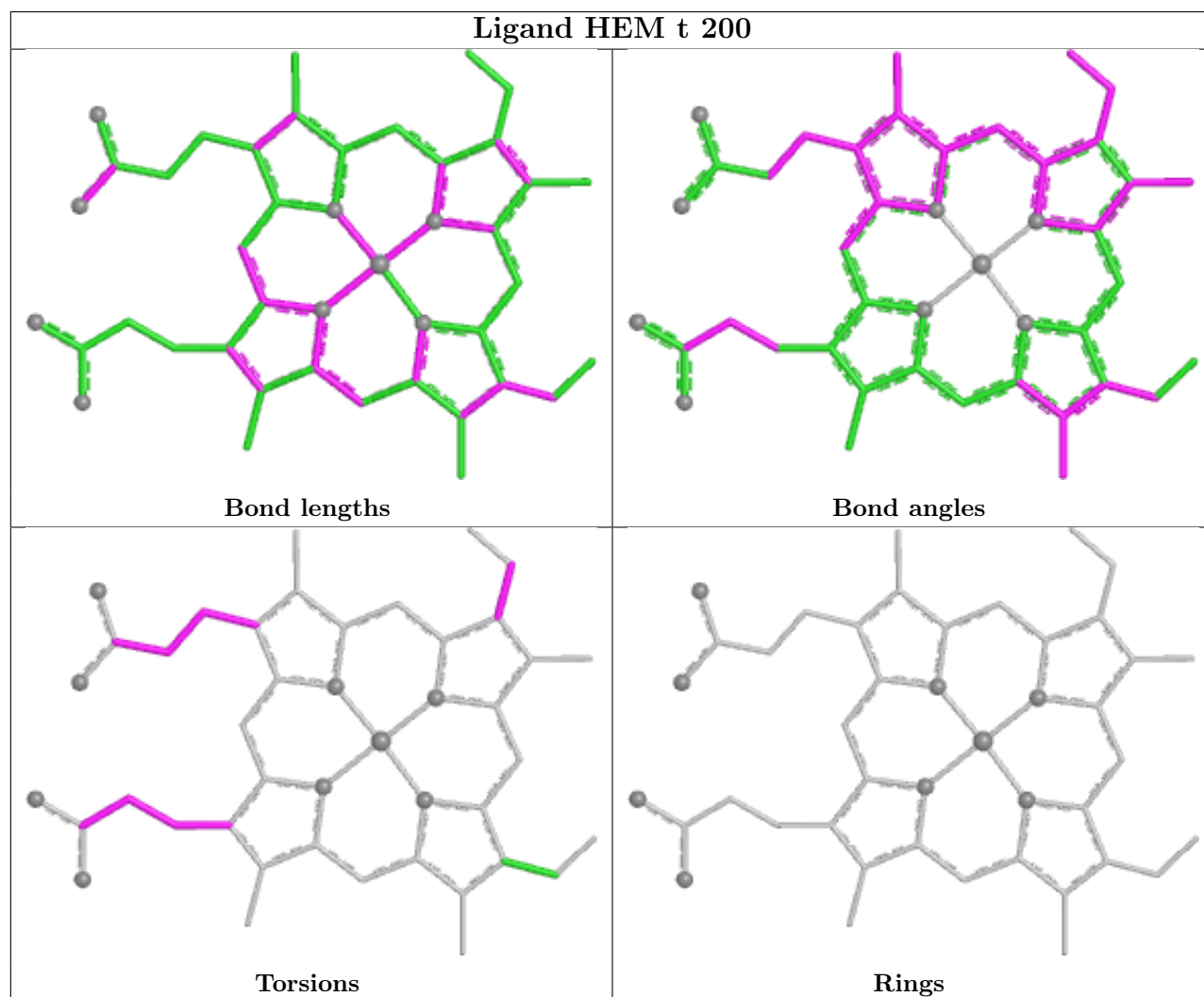
There are no ring outliers.

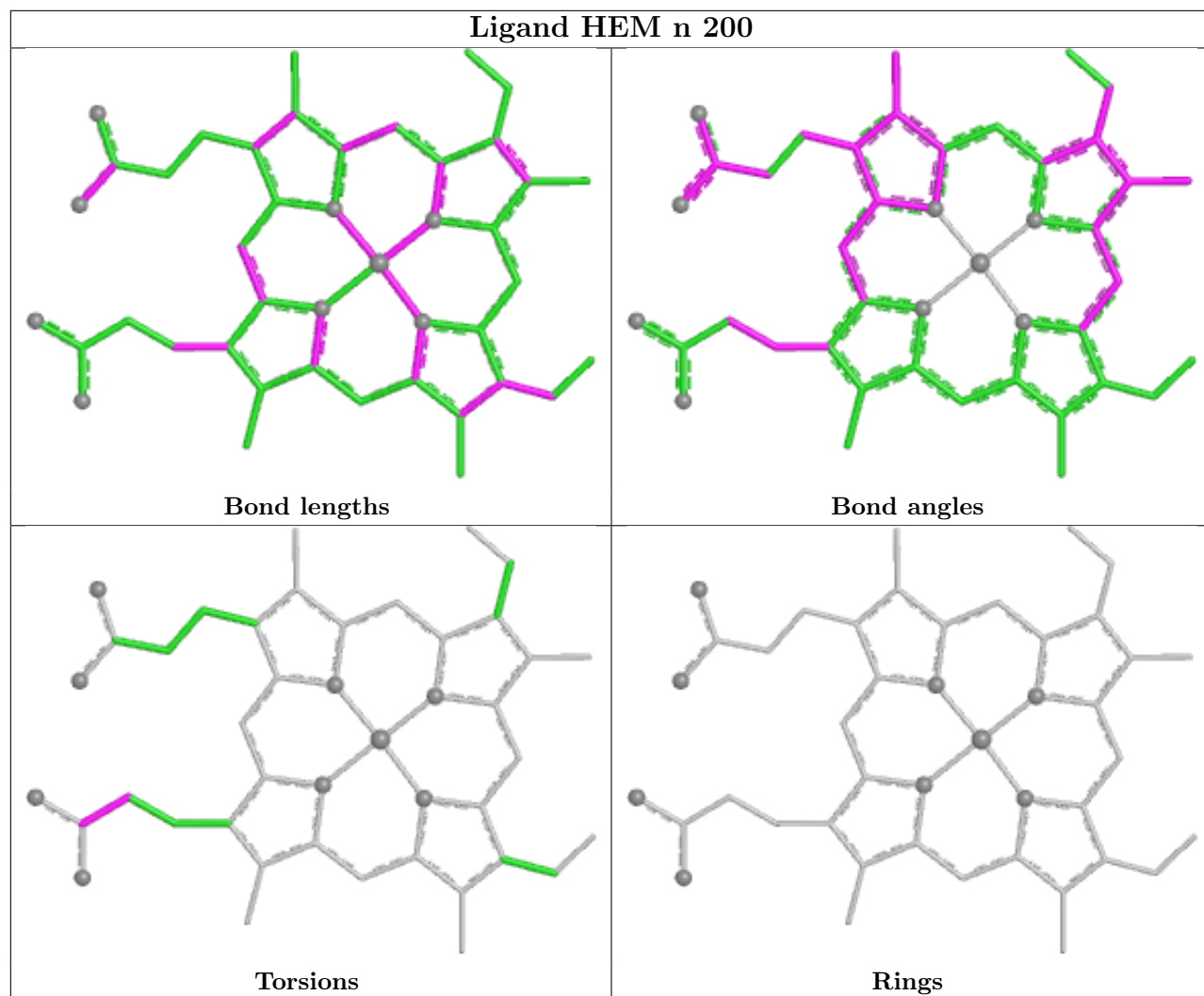
24 monomers are involved in 209 short contacts:

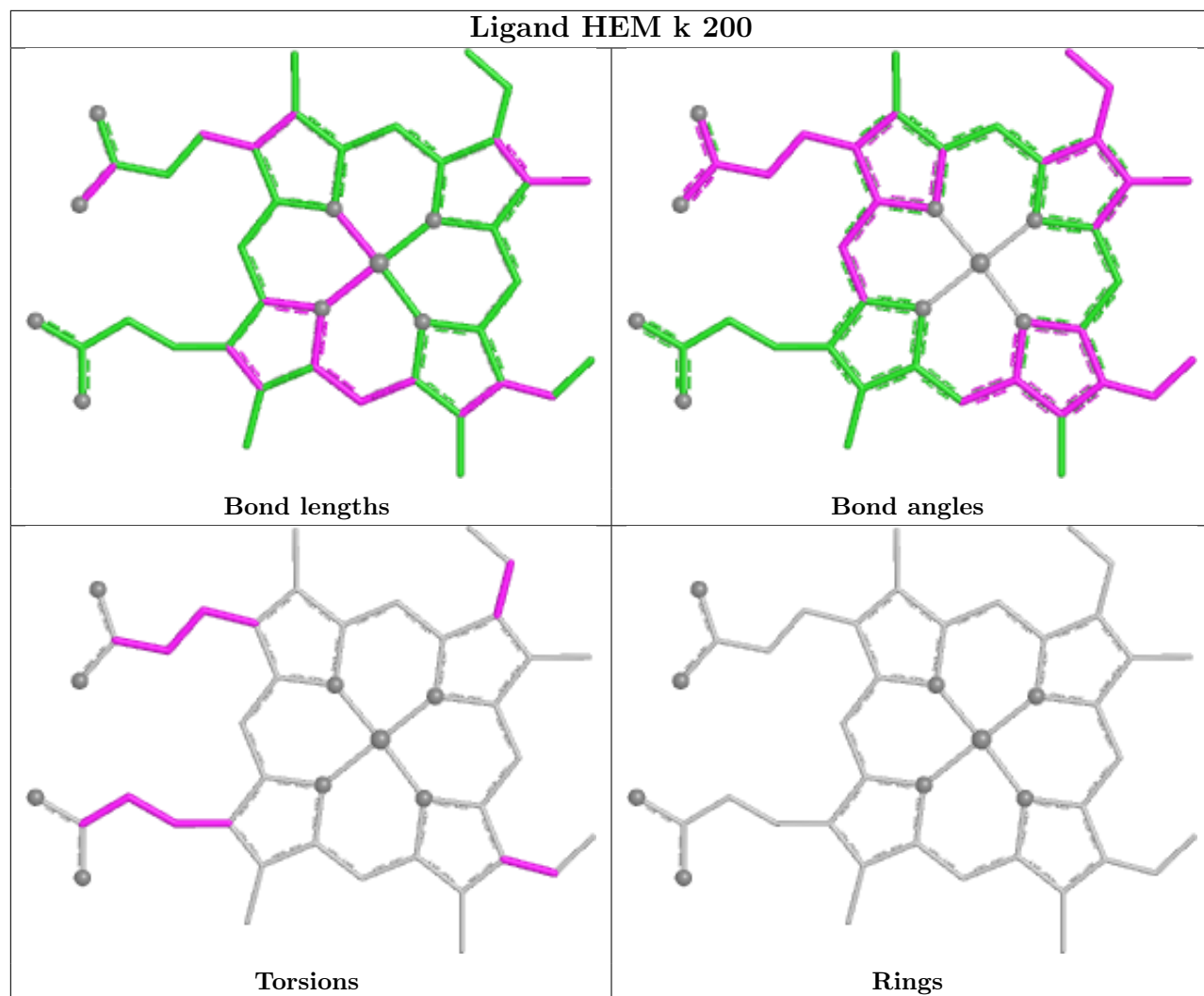
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	t	200	HEM	13	0
2	n	200	HEM	6	0
2	k	200	HEM	12	0
2	v	200	HEM	3	0
2	U	200	HEM	4	0
2	P	200	HEM	9	0
2	M	200	HEM	8	0
2	C	200	HEM	23	0
2	g	200	HEM	11	0
2	B	200	HEM	8	0
2	q	200	HEM	16	0
2	I	200	HEM	5	0
2	e	200	HEM	9	0
2	F	200	HEM	4	0
2	o	200	HEM	8	0
2	L	200	HEM	12	0
2	c	200	HEM	6	0
2	x	200	HEM	9	0
2	S	200	HEM	5	0
2	H	200	HEM	7	0
2	X	200	HEM	6	0
2	R	200	HEM	14	0
2	a	200	HEM	5	0
2	j	200	HEM	6	0

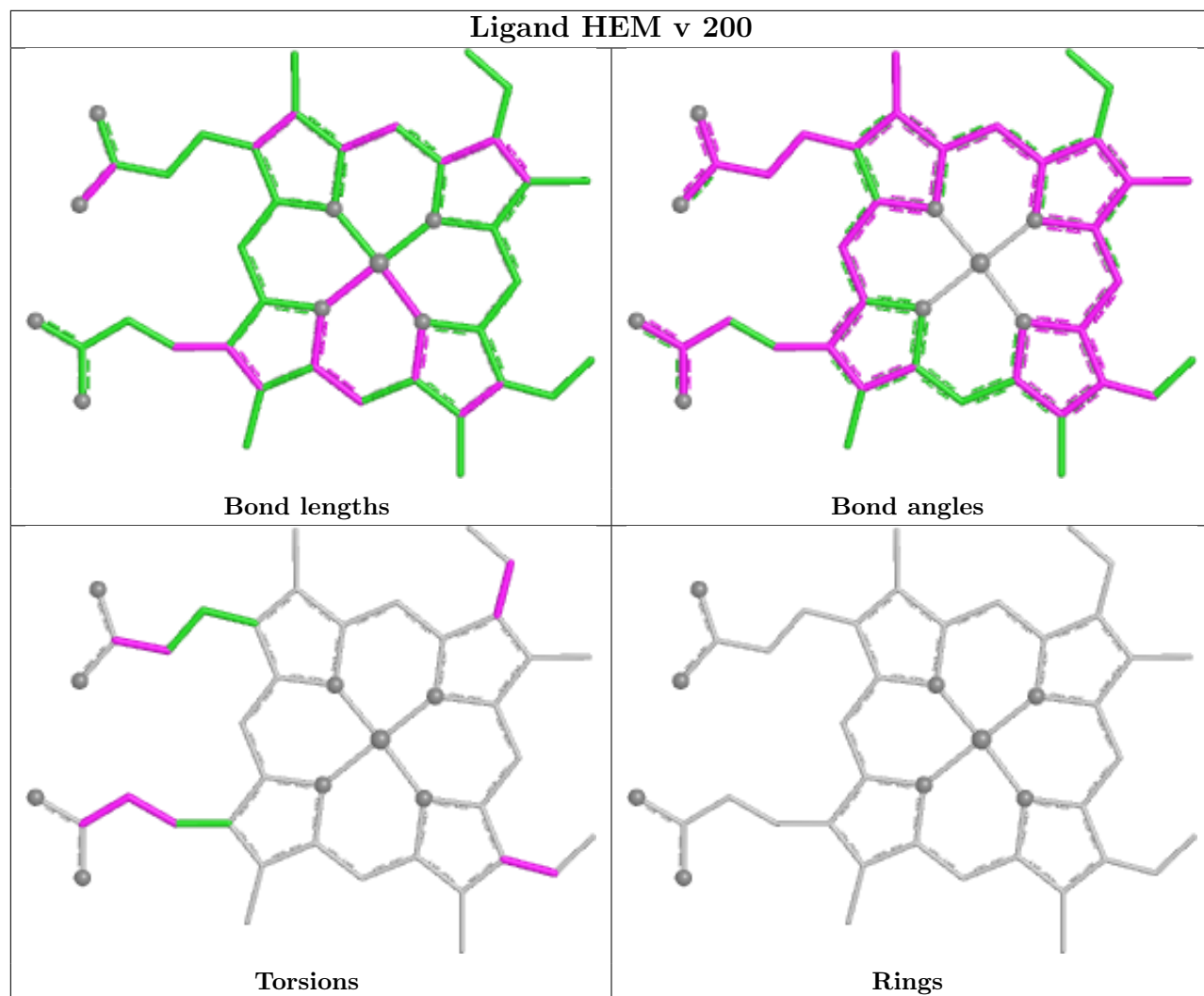
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

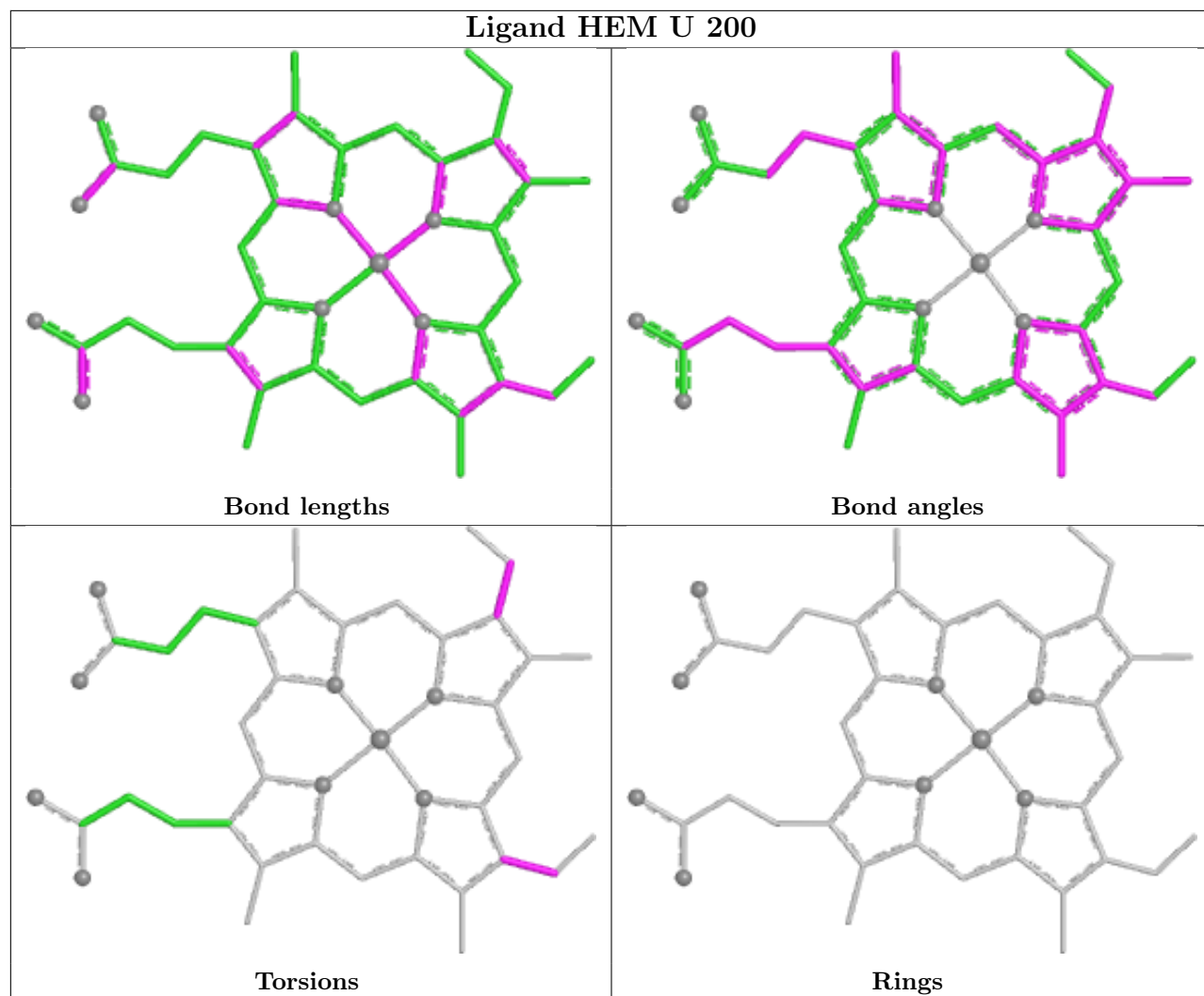
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

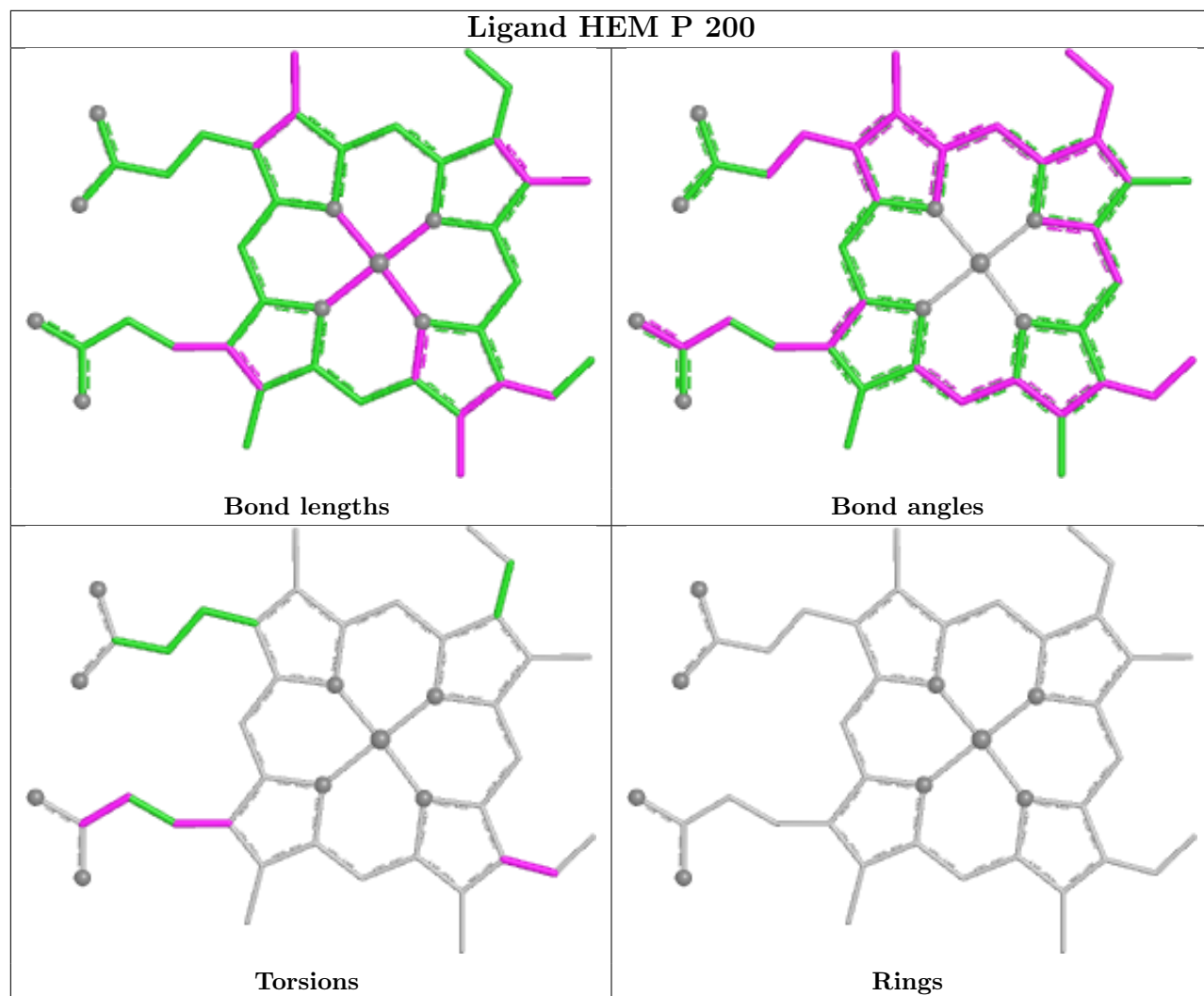




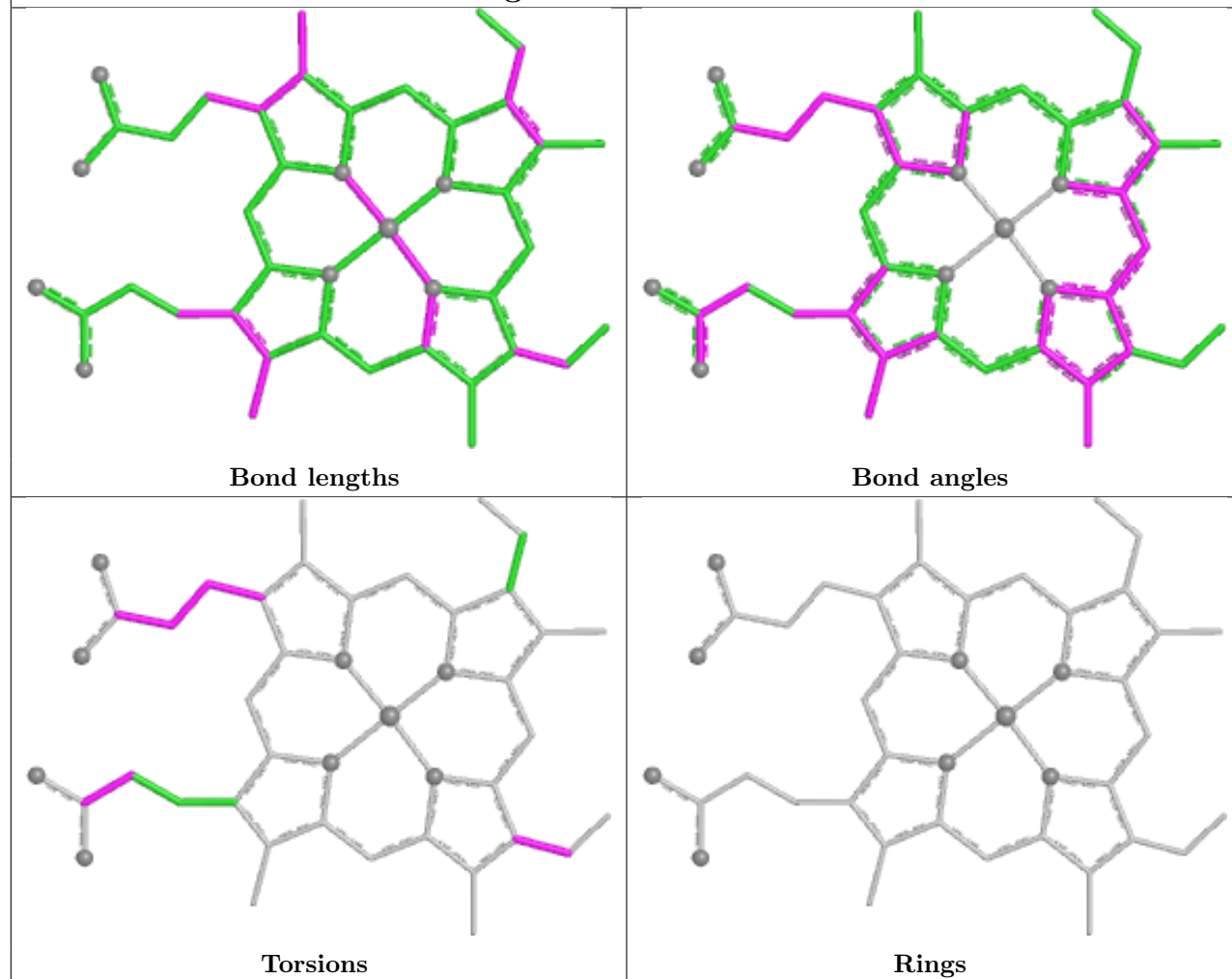


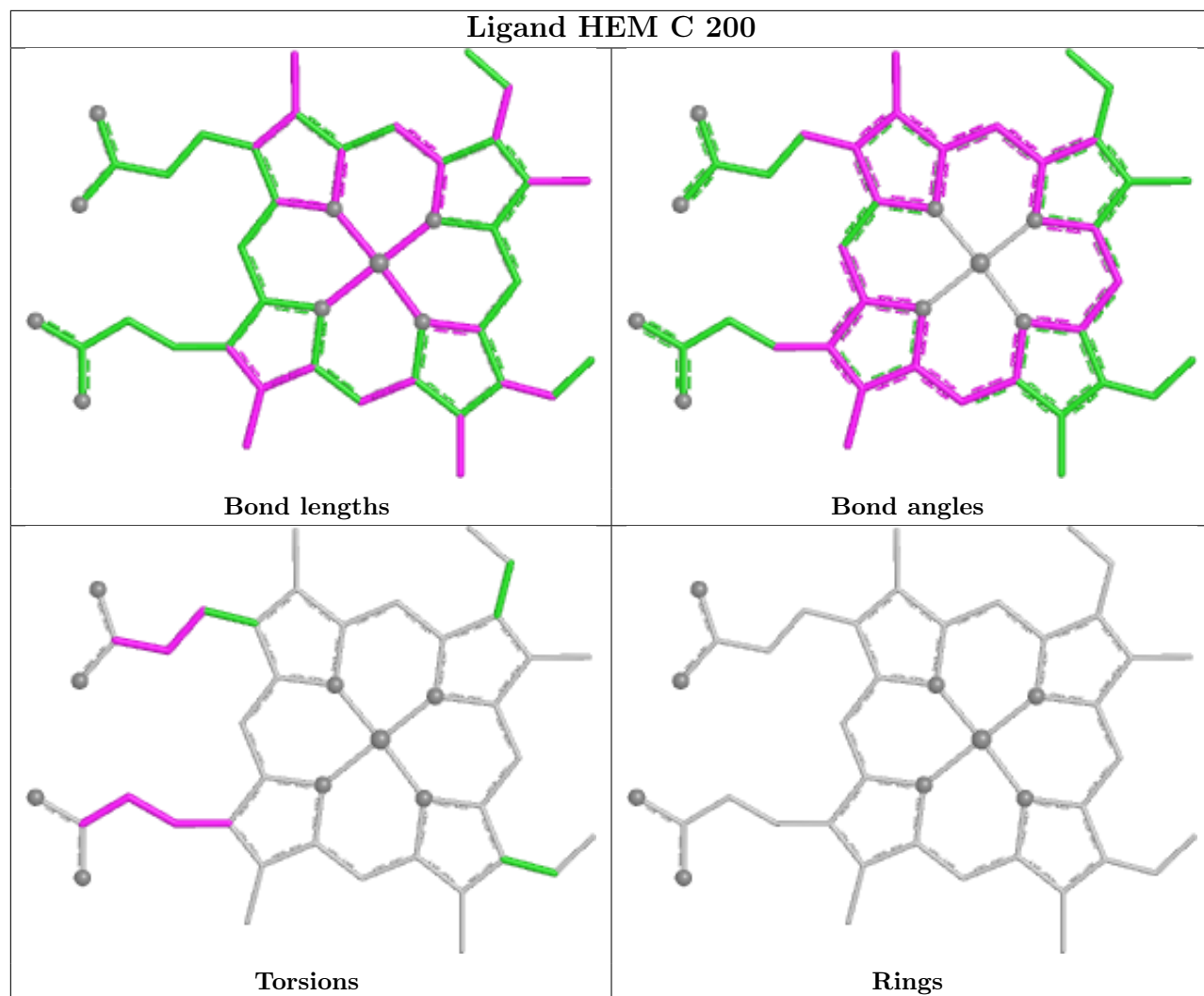


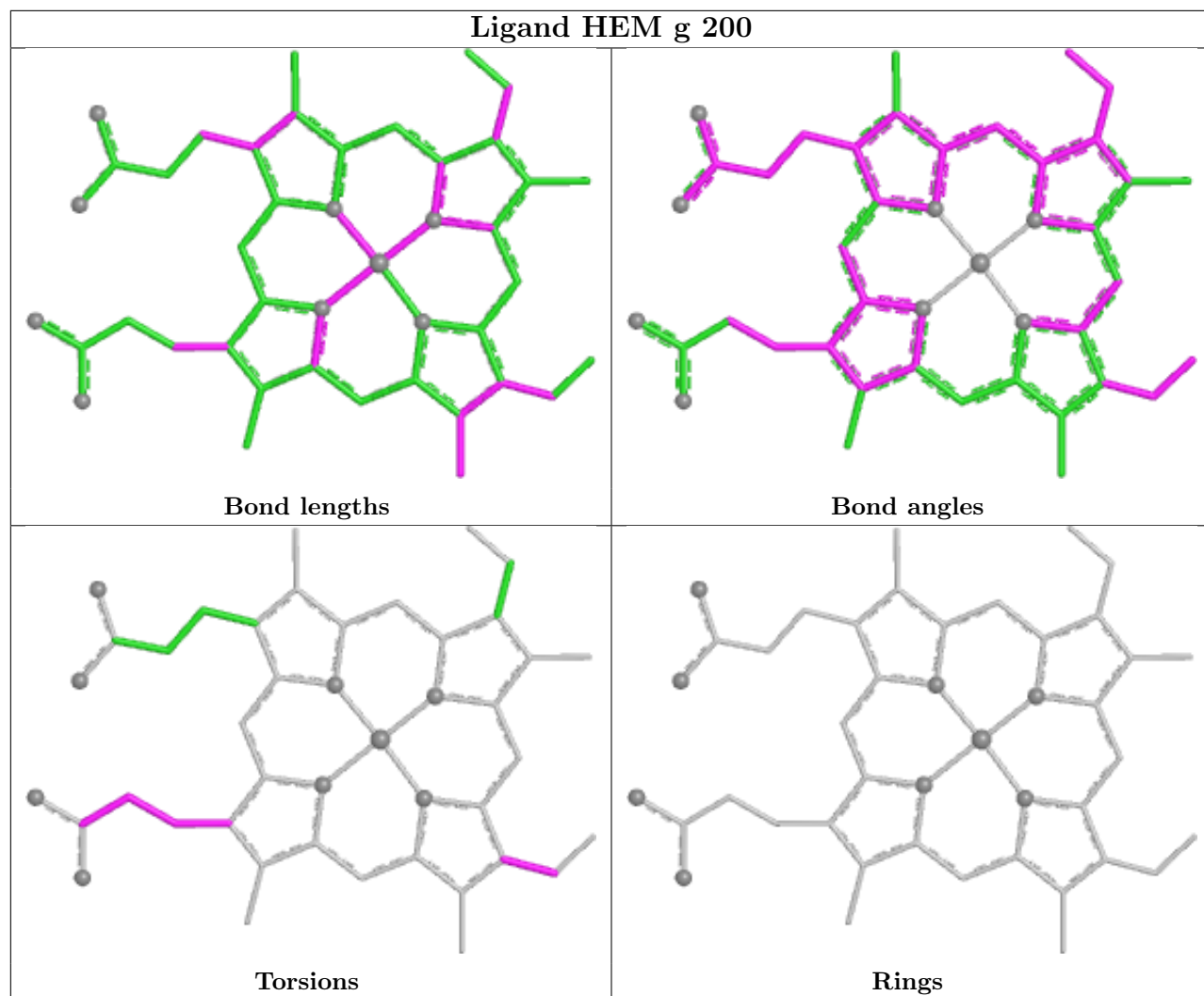


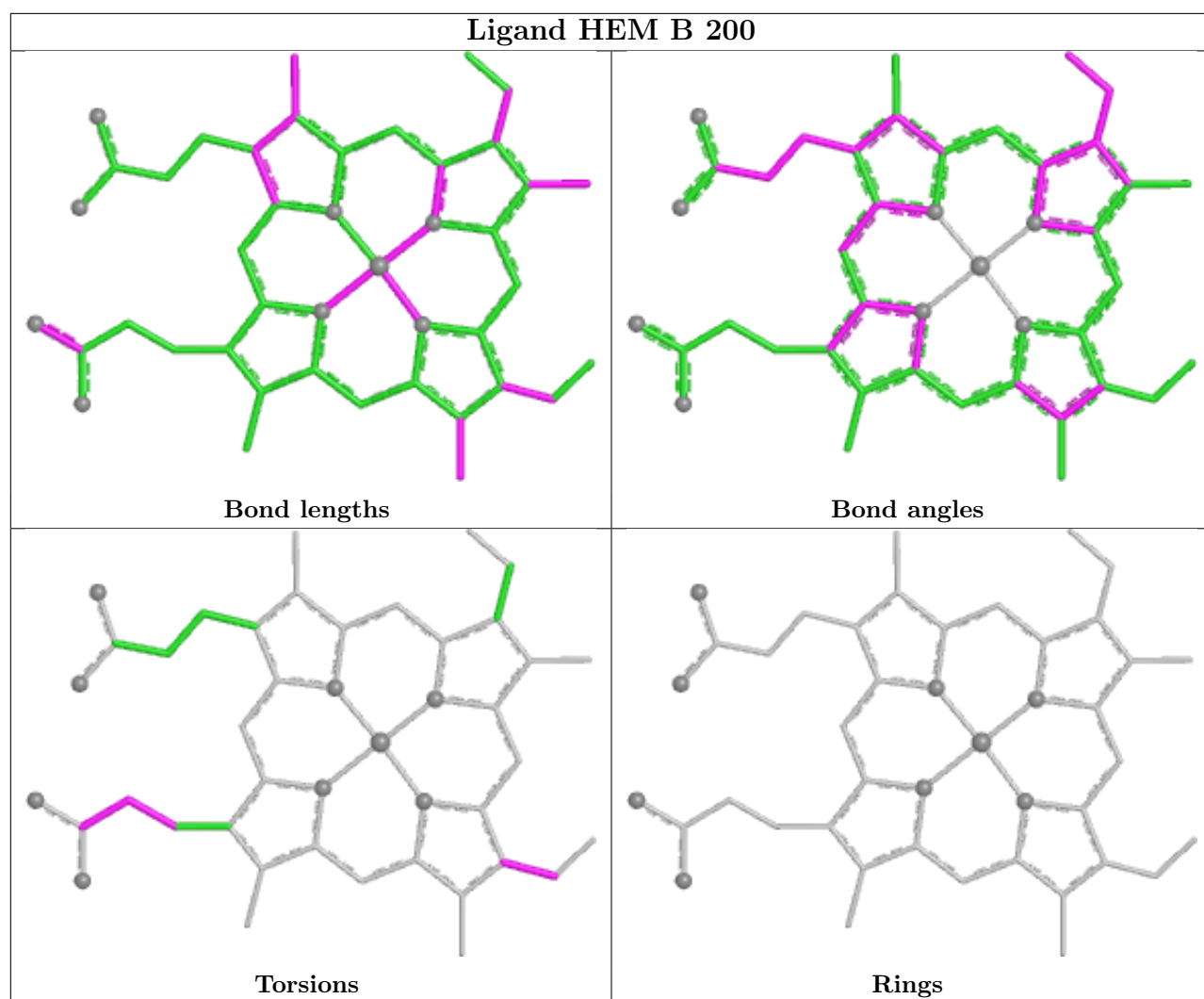


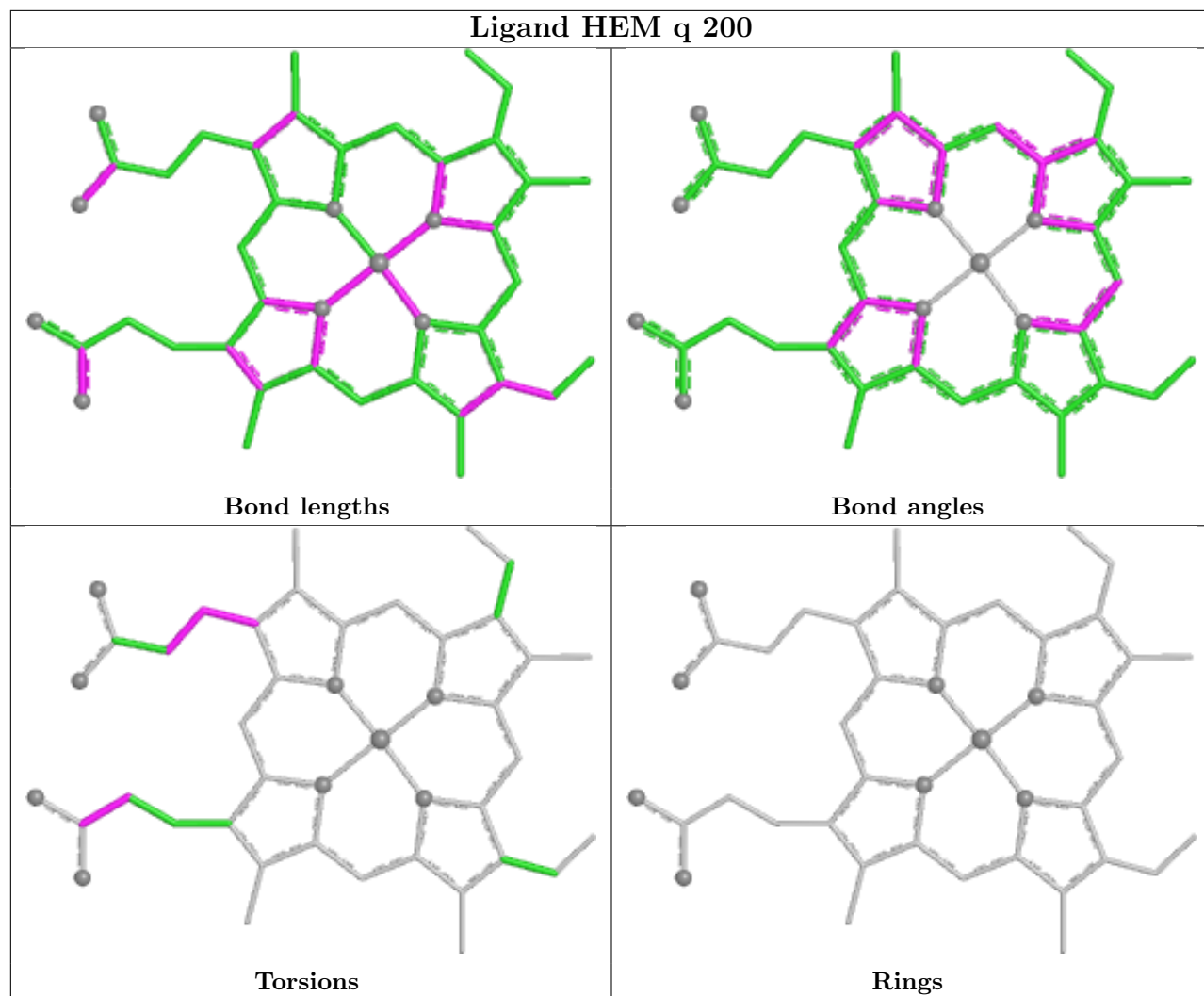
Ligand HEM M 200



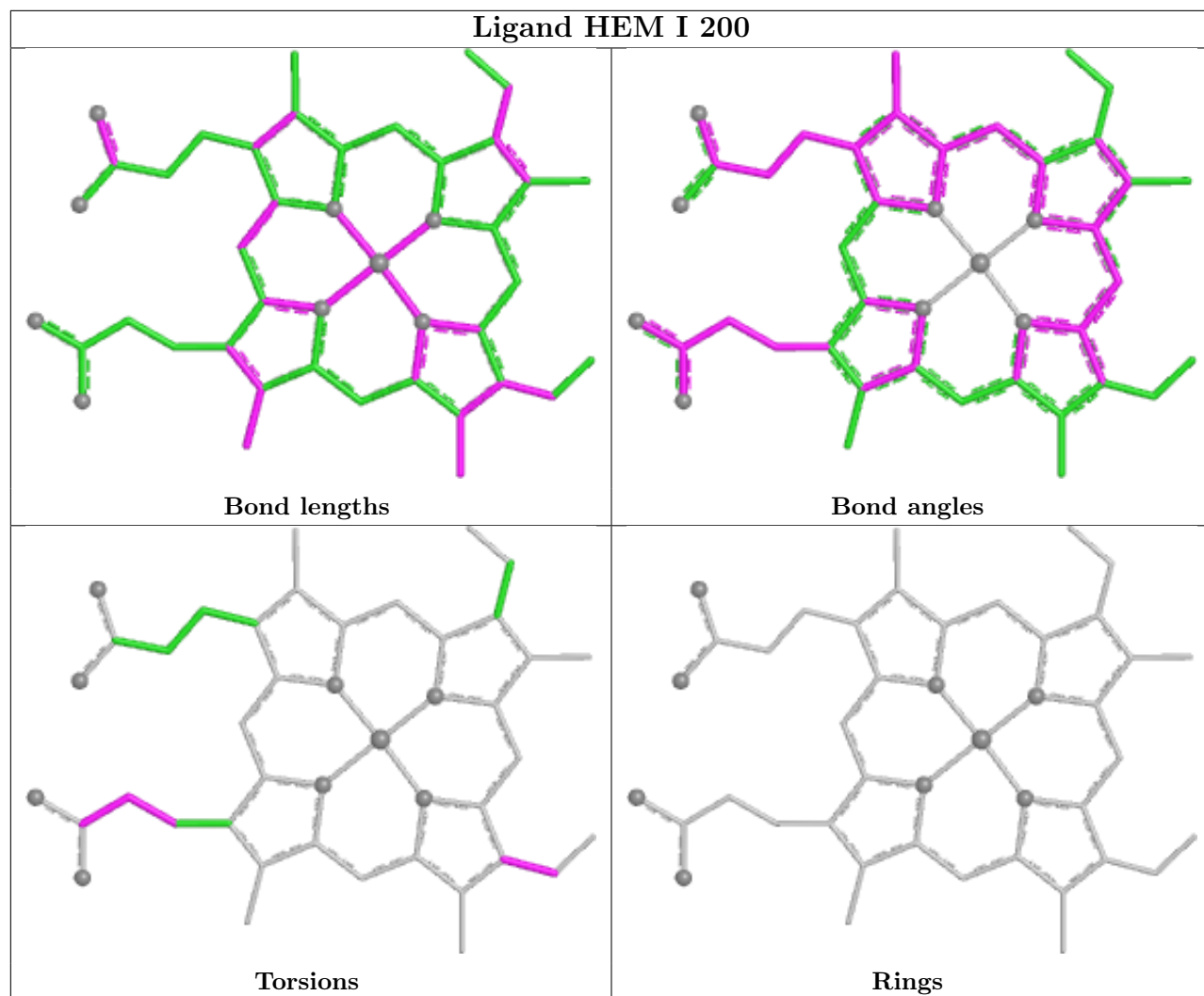




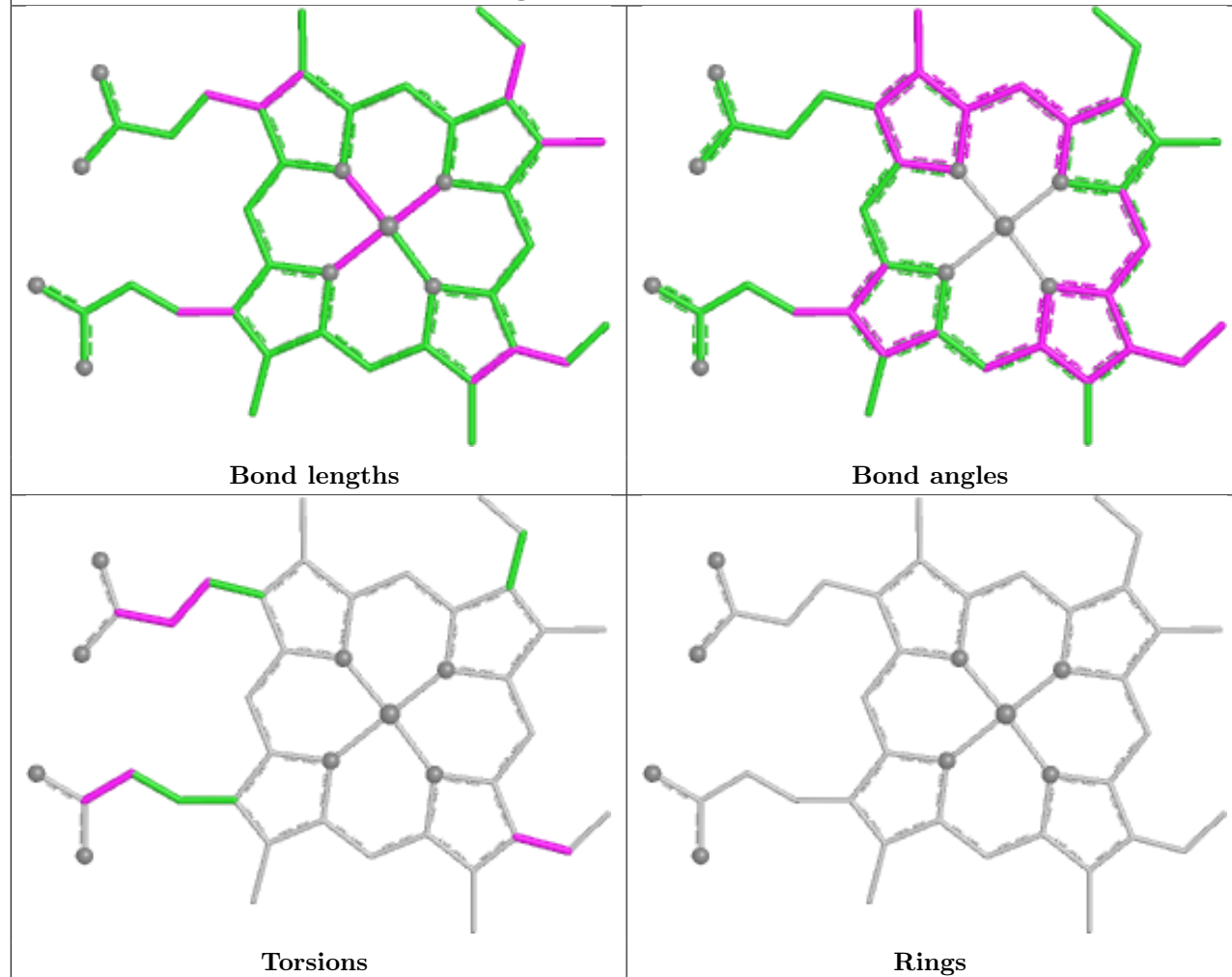


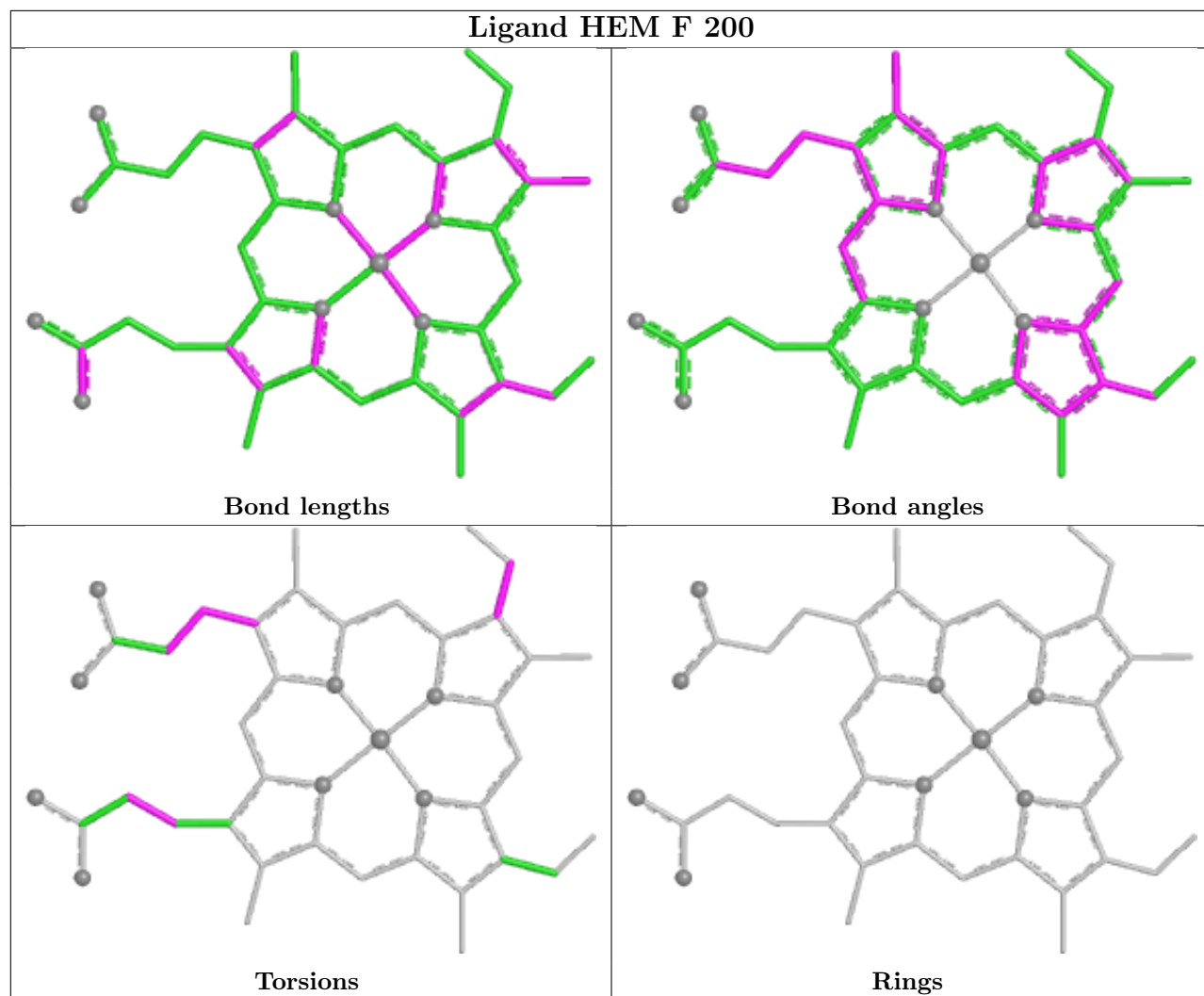


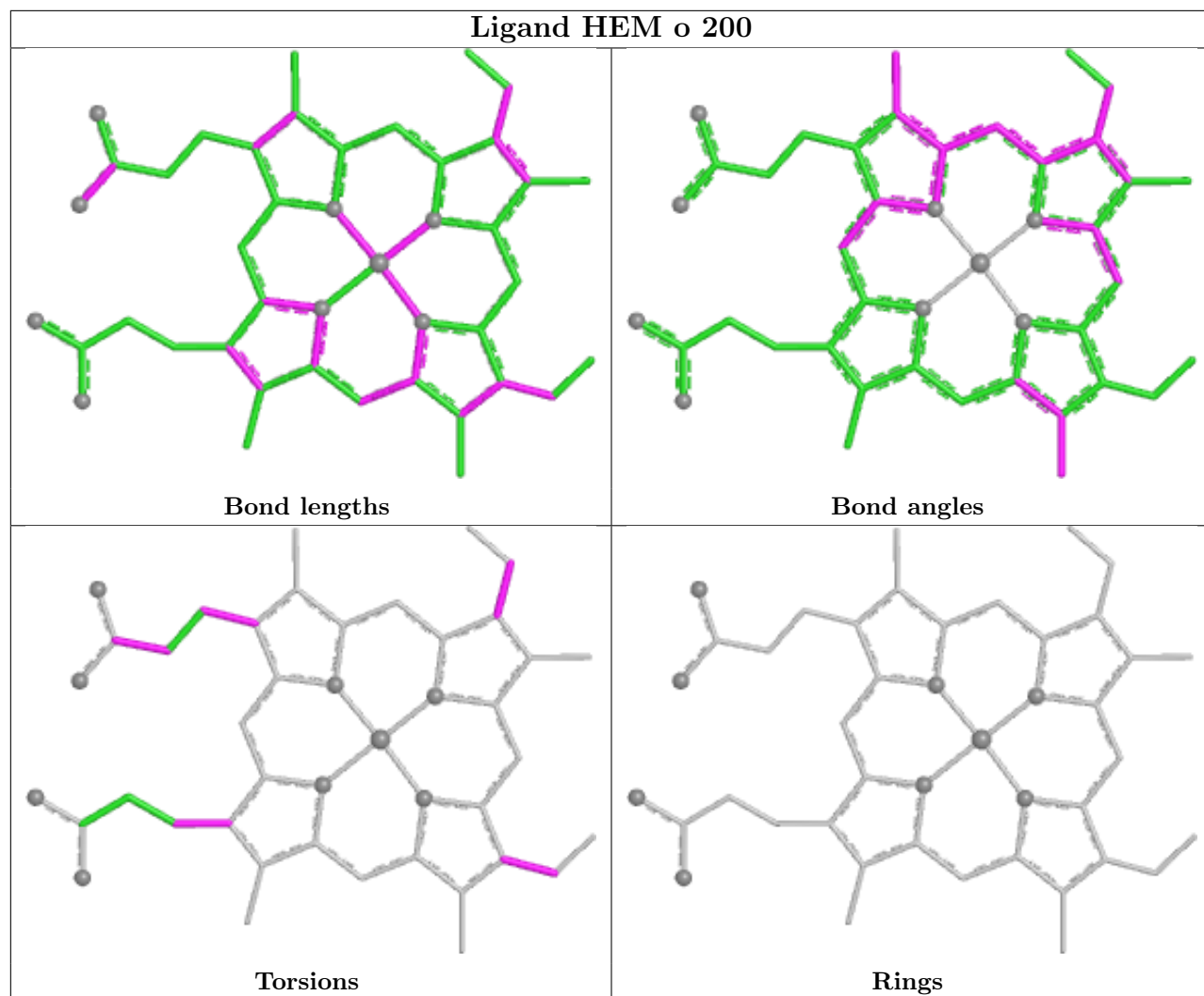
Ligand HEM I 200

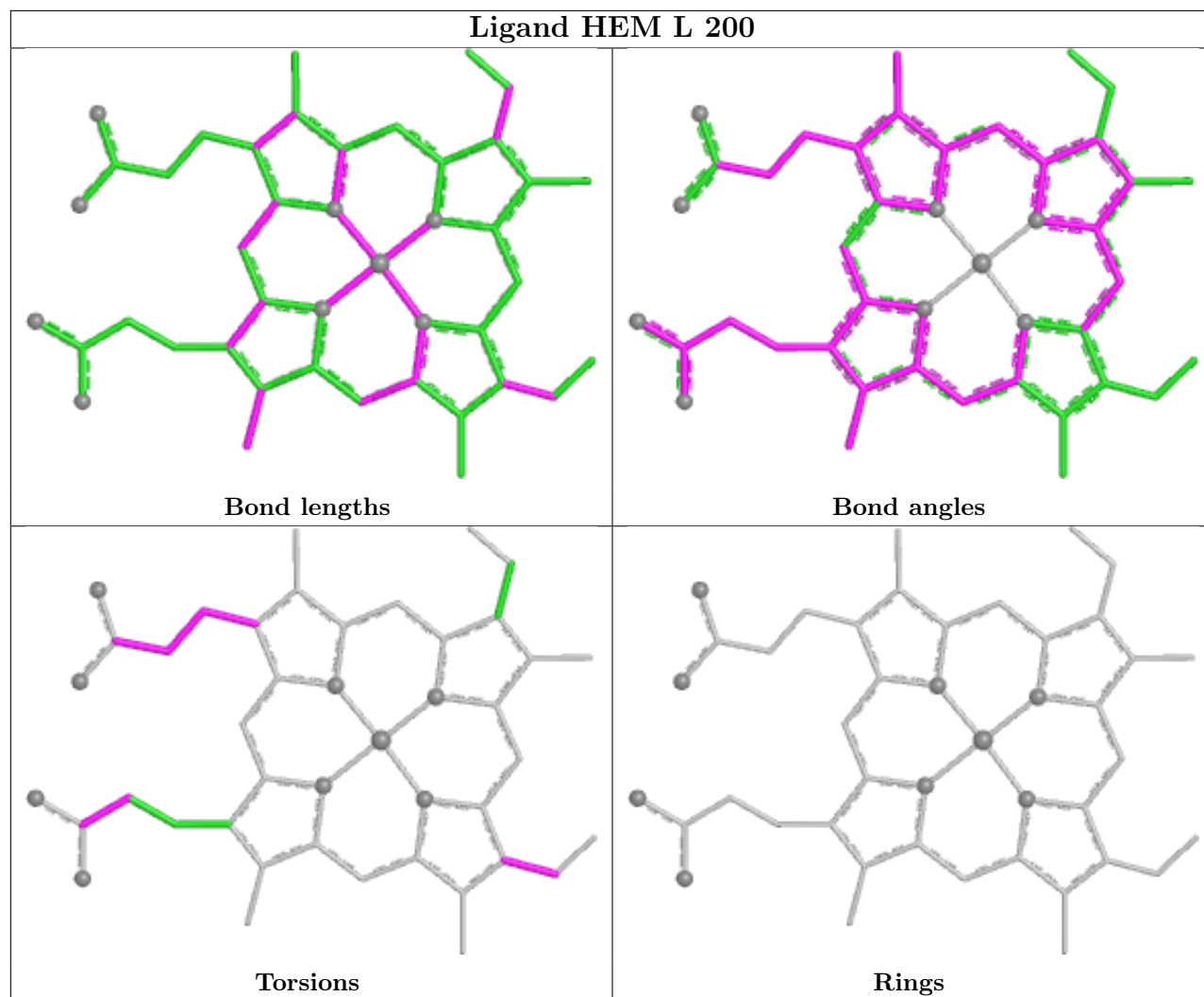


Ligand HEM e 200

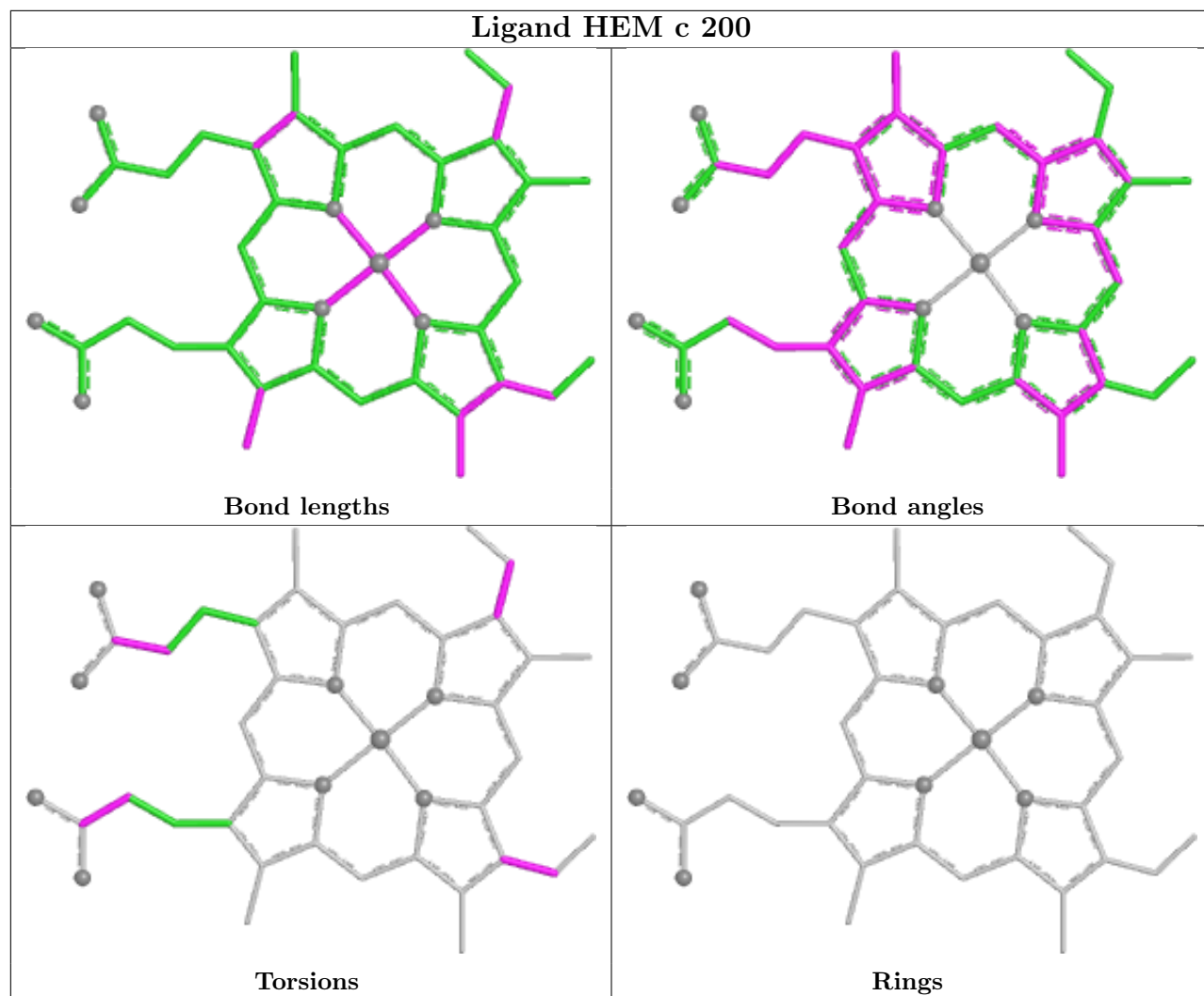


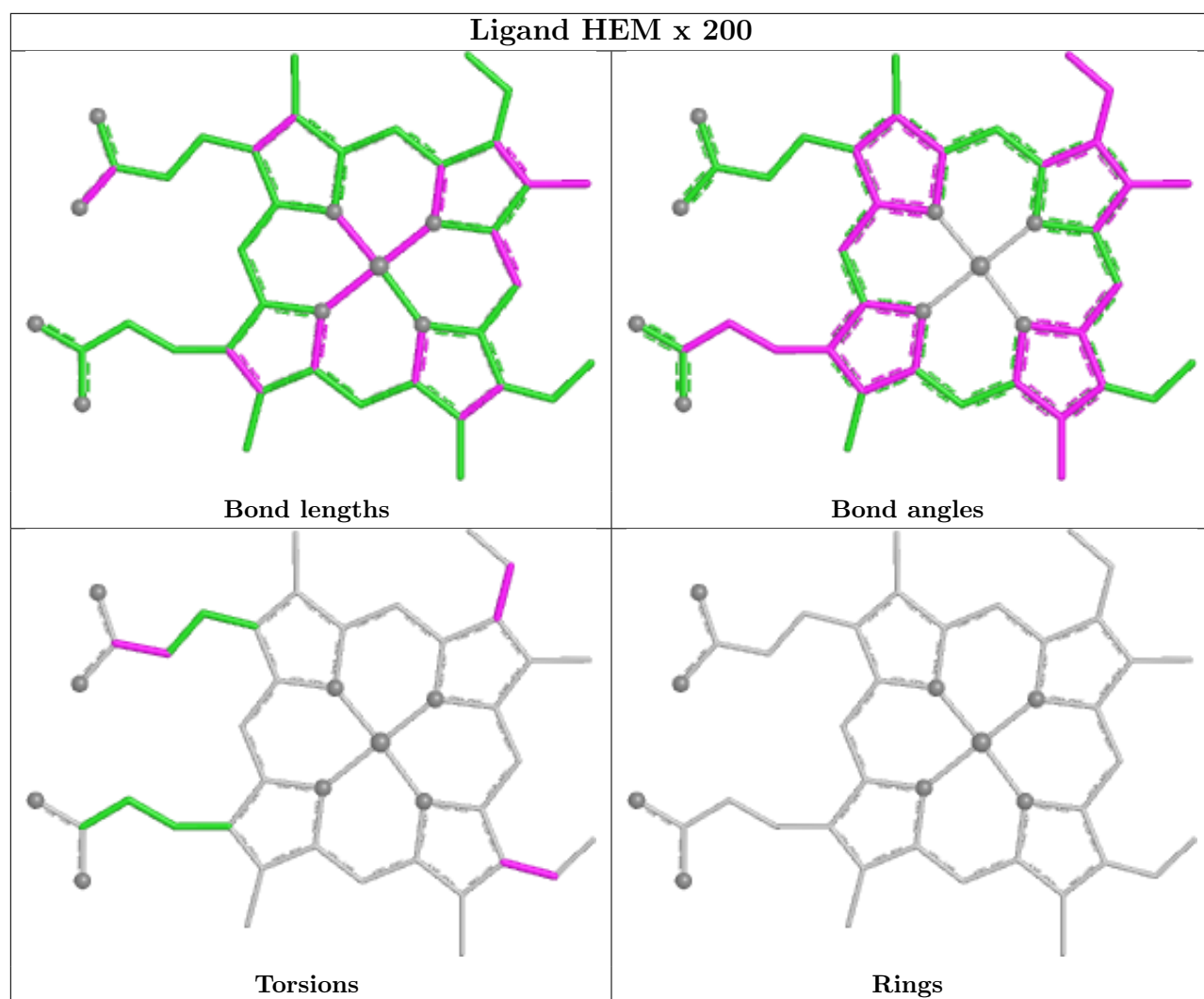


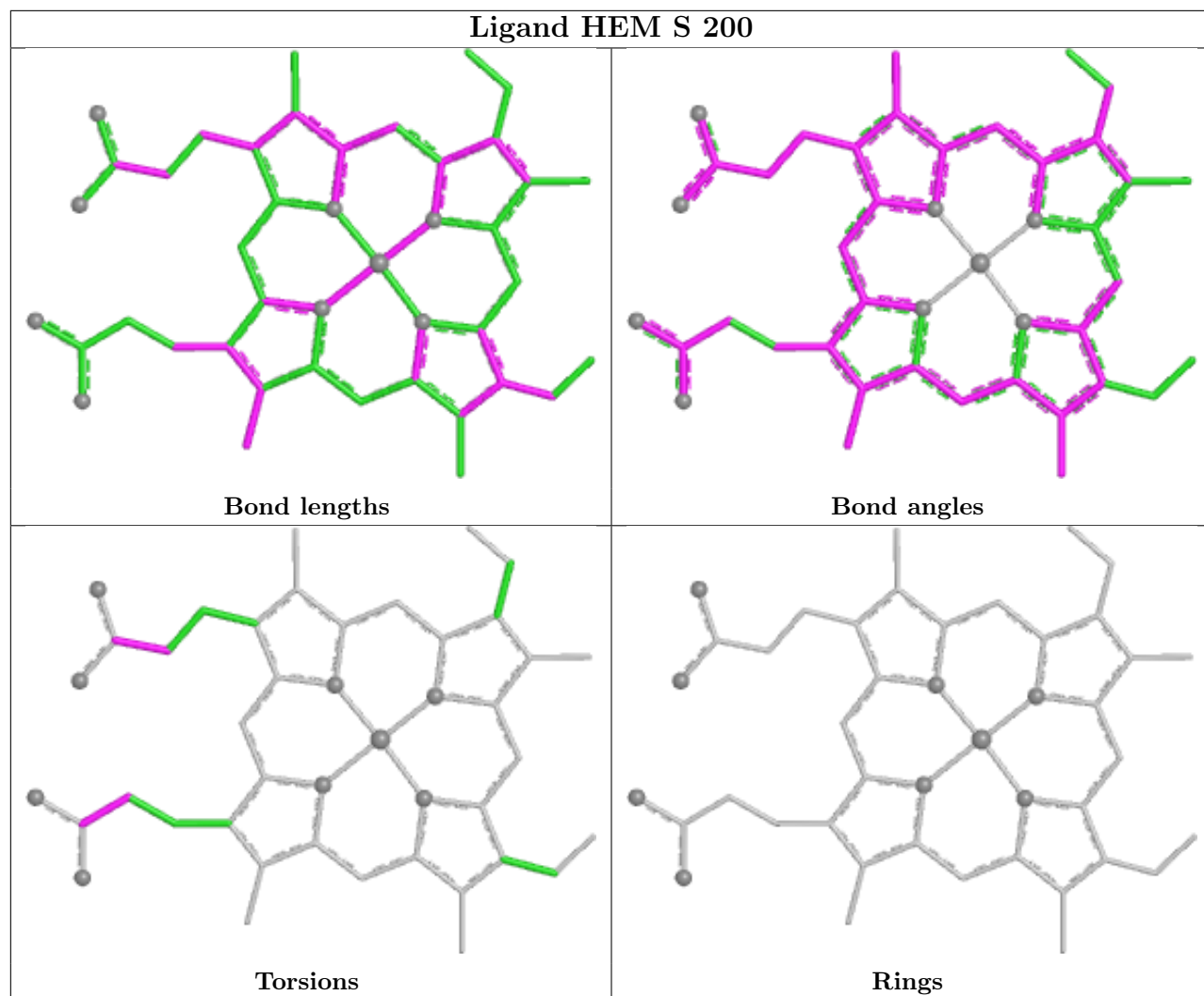


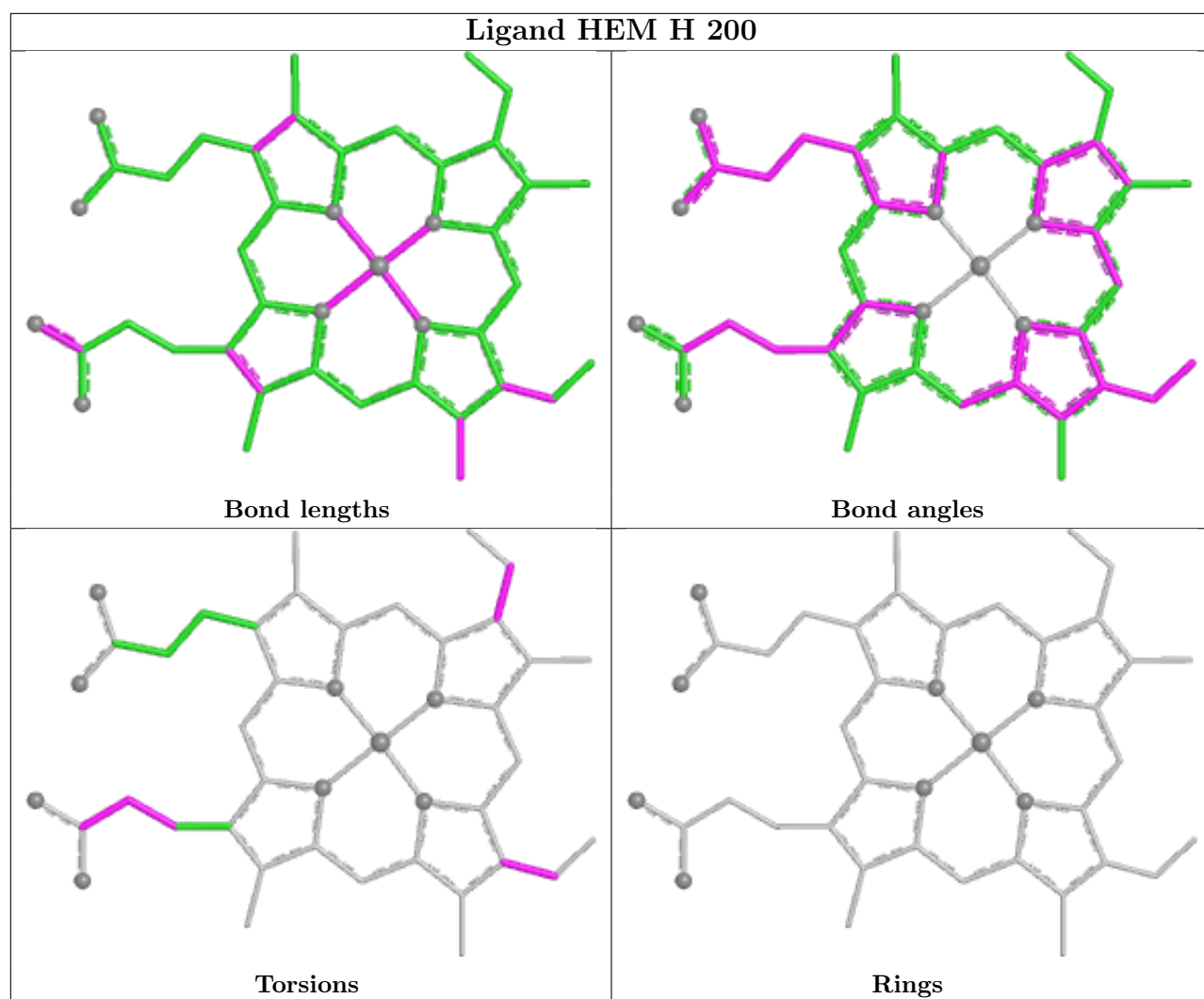


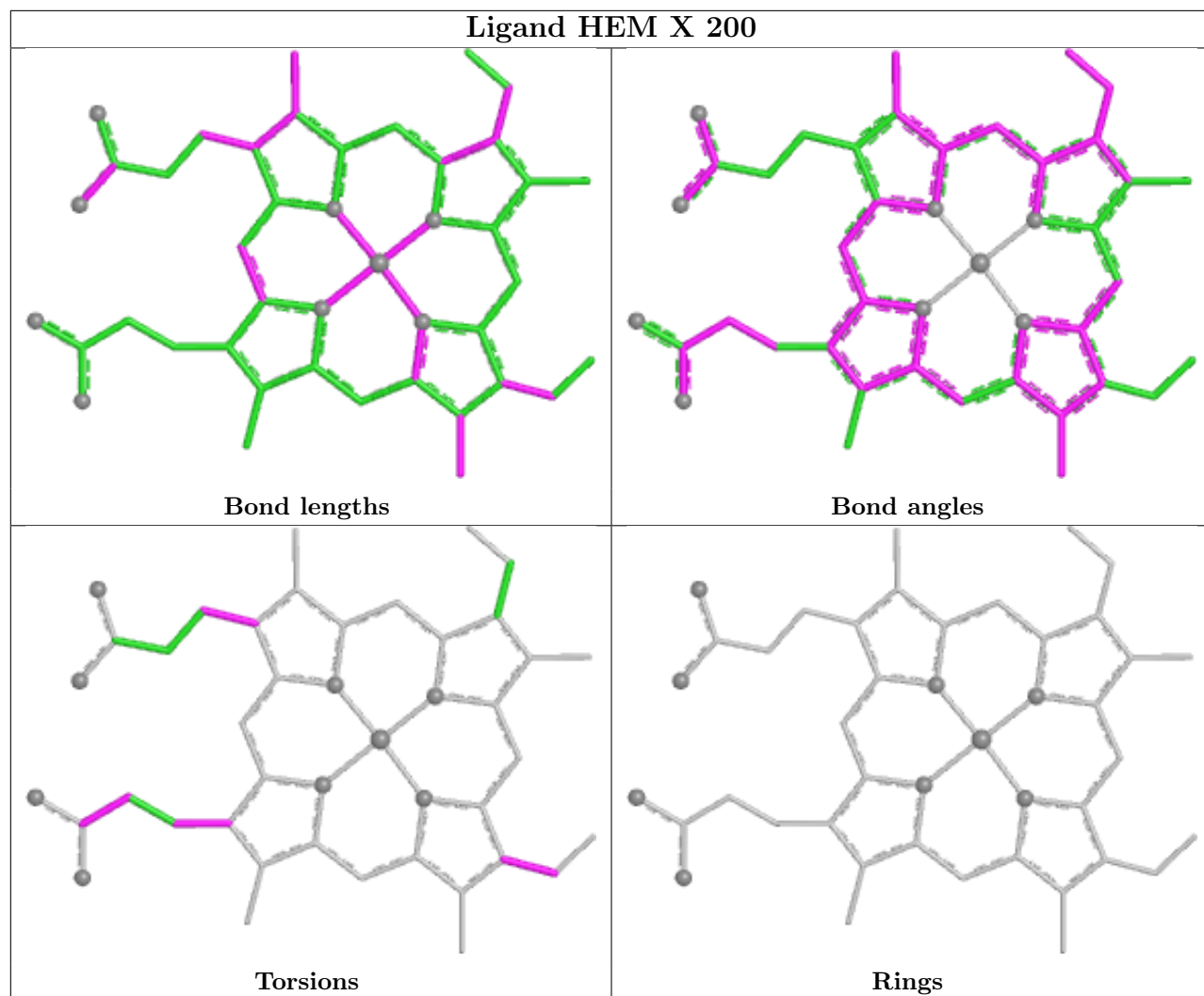
Ligand HEM c 200

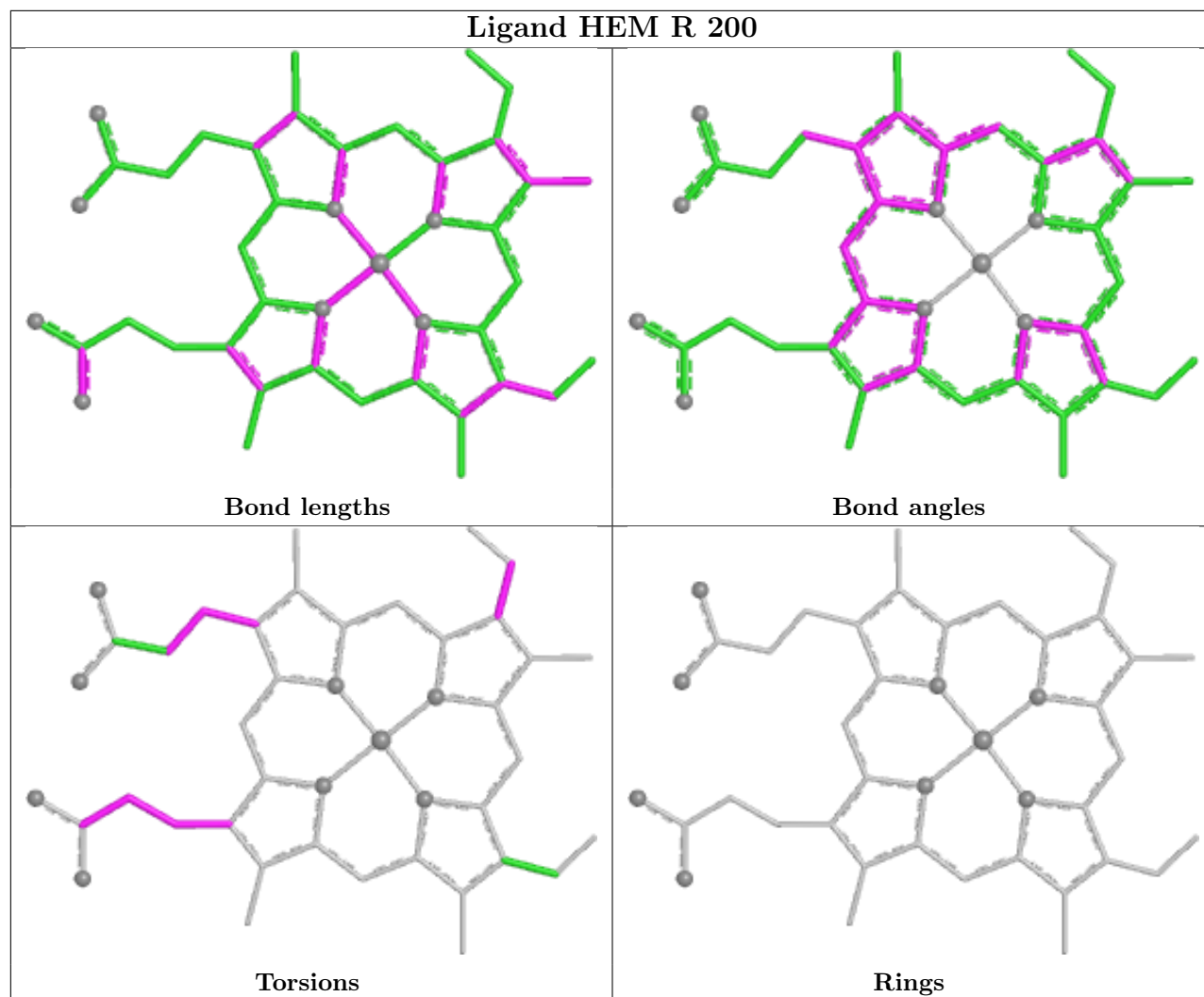


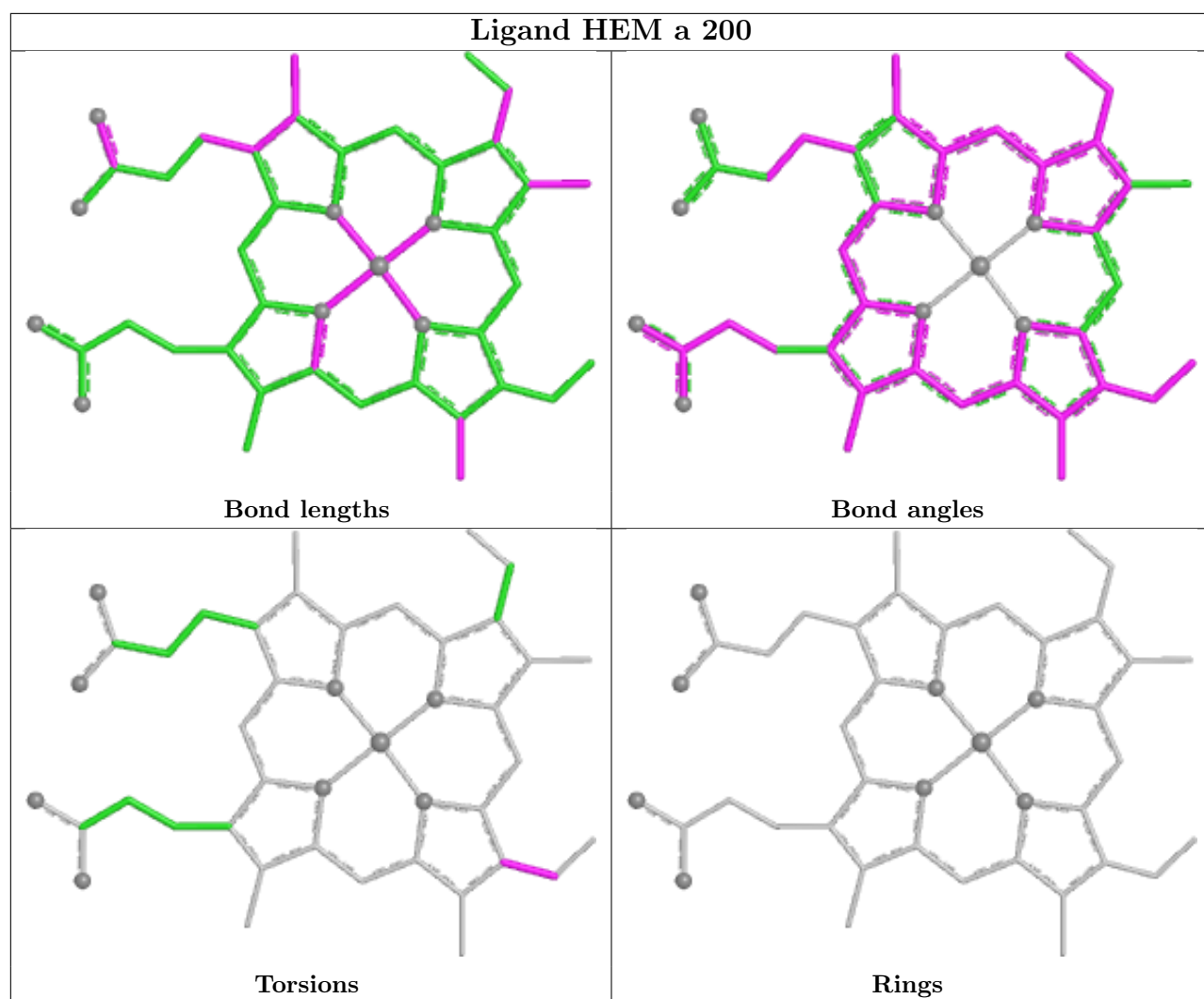


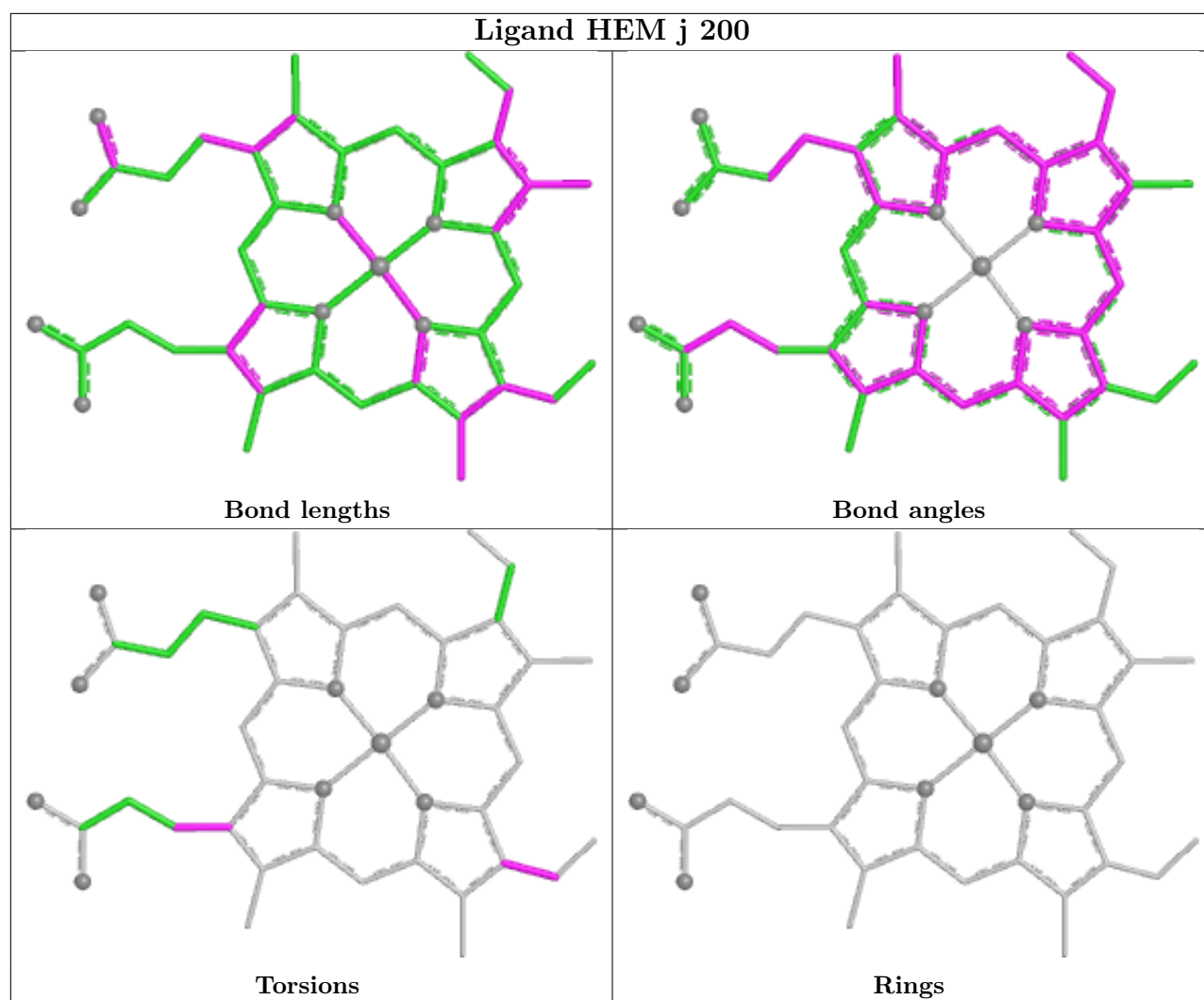












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	159/161 (98%)	-1.27	0 100 100	16, 24, 32, 39	0
1	B	159/161 (98%)	-1.26	0 100 100	15, 25, 33, 41	0
1	C	159/161 (98%)	-1.20	0 100 100	16, 25, 33, 39	0
1	D	159/161 (98%)	-1.23	0 100 100	16, 24, 33, 43	0
1	E	159/161 (98%)	-1.15	0 100 100	16, 25, 34, 42	0
1	F	159/161 (98%)	-1.22	0 100 100	16, 24, 32, 39	0
1	G	159/161 (98%)	-1.26	0 100 100	16, 23, 32, 36	0
1	H	159/161 (98%)	-1.25	0 100 100	12, 22, 30, 41	0
1	I	159/161 (98%)	-1.31	0 100 100	14, 22, 31, 36	0
1	J	159/161 (98%)	-1.30	0 100 100	14, 22, 30, 41	0
1	K	159/161 (98%)	-1.26	0 100 100	15, 25, 33, 37	0
1	L	159/161 (98%)	-1.26	0 100 100	14, 24, 33, 42	0
1	M	159/161 (98%)	-1.25	0 100 100	17, 26, 34, 45	0
1	N	159/161 (98%)	-1.27	0 100 100	17, 24, 34, 39	0
1	O	159/161 (98%)	-1.31	0 100 100	16, 22, 31, 40	0
1	P	159/161 (98%)	-1.32	0 100 100	13, 23, 31, 38	0
1	Q	159/161 (98%)	-1.14	0 100 100	16, 26, 36, 44	0
1	R	159/161 (98%)	-1.18	0 100 100	16, 24, 32, 46	0
1	S	159/161 (98%)	-1.31	0 100 100	13, 20, 29, 35	0
1	T	159/161 (98%)	-1.35	0 100 100	12, 20, 28, 42	0
1	U	159/161 (98%)	-1.31	0 100 100	13, 21, 30, 39	0
1	V	159/161 (98%)	-1.30	0 100 100	15, 22, 30, 36	0
1	W	159/161 (98%)	-1.20	0 100 100	17, 26, 35, 42	0
1	X	159/161 (98%)	-1.28	0 100 100	14, 23, 31, 44	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)	Q<0.9		
1	a	159/161 (98%)	-1.33	0	100	100	13, 22, 31, 38	0
1	b	159/161 (98%)	-1.24	0	100	100	14, 23, 32, 40	0
1	c	159/161 (98%)	-1.25	0	100	100	17, 25, 34, 40	0
1	d	159/161 (98%)	-1.24	0	100	100	17, 25, 34, 43	0
1	e	159/161 (98%)	-1.20	0	100	100	20, 28, 36, 46	0
1	f	159/161 (98%)	-1.21	0	100	100	17, 25, 34, 42	0
1	g	159/161 (98%)	-1.25	0	100	100	15, 24, 32, 39	0
1	h	159/161 (98%)	-1.29	0	100	100	16, 23, 32, 42	0
1	i	159/161 (98%)	-1.29	0	100	100	15, 22, 34, 38	0
1	j	159/161 (98%)	-1.32	0	100	100	14, 22, 30, 39	0
1	k	159/161 (98%)	-1.23	0	100	100	14, 23, 33, 38	0
1	l	159/161 (98%)	-1.28	0	100	100	14, 23, 32, 39	0
1	m	159/161 (98%)	-1.28	0	100	100	15, 22, 33, 38	0
1	n	159/161 (98%)	-1.27	0	100	100	15, 23, 32, 42	0
1	o	159/161 (98%)	-1.31	0	100	100	16, 24, 30, 36	0
1	p	159/161 (98%)	-1.29	0	100	100	18, 24, 31, 41	0
1	q	159/161 (98%)	-1.20	0	100	100	20, 28, 36, 43	0
1	r	159/161 (98%)	-1.20	0	100	100	18, 27, 36, 43	0
1	s	159/161 (98%)	-1.31	0	100	100	14, 23, 31, 37	0
1	t	159/161 (98%)	-1.34	0	100	100	14, 21, 30, 34	0
1	u	159/161 (98%)	-1.33	0	100	100	13, 21, 29, 37	0
1	v	159/161 (98%)	-1.34	0	100	100	14, 22, 32, 39	0
1	w	159/161 (98%)	-1.21	0	100	100	16, 25, 34, 44	0
1	x	159/161 (98%)	-1.26	0	100	100	14, 21, 29, 38	0
All	All	7632/7728 (98%)	-1.26	0	100	100	12, 24, 33, 46	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

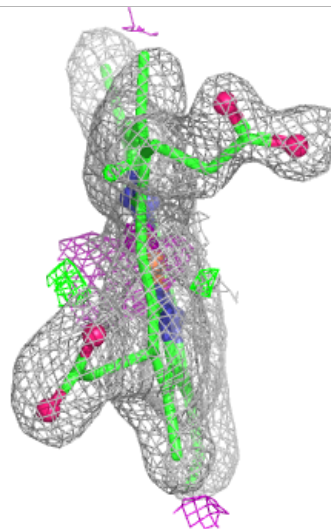
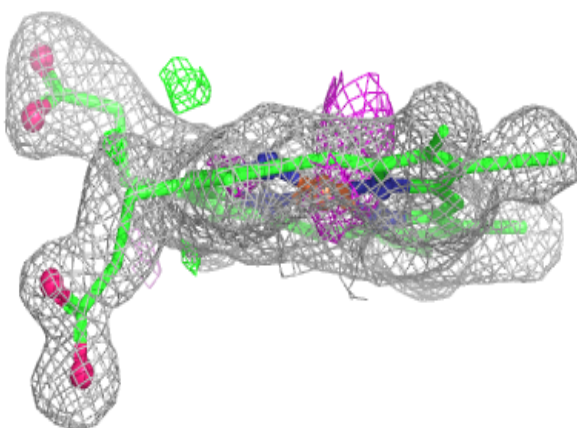
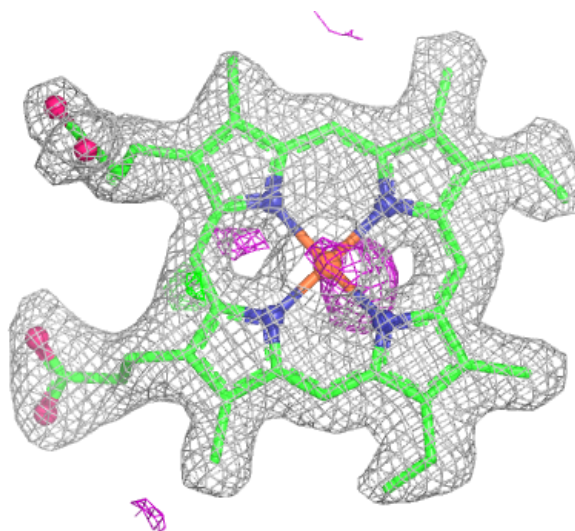
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	B	200	43/43	0.99	0.04	18,27,38,45	0
2	HEM	C	200	43/43	0.99	0.04	18,31,44,47	0
2	HEM	F	200	43/43	0.99	0.04	16,28,46,52	0
2	HEM	H	200	43/43	0.99	0.03	14,24,32,35	0
2	HEM	I	200	43/43	0.99	0.03	10,21,34,37	0
2	HEM	P	200	43/43	0.99	0.04	12,25,37,39	0
2	HEM	R	200	43/43	0.99	0.04	21,28,38,40	0
2	HEM	U	200	43/43	0.99	0.03	10,20,26,33	0
2	HEM	X	200	43/43	0.99	0.03	13,24,37,41	0
2	HEM	a	200	43/43	0.99	0.04	13,22,29,33	0
2	HEM	c	200	43/43	0.99	0.04	17,27,40,43	0
2	HEM	e	200	43/43	0.99	0.04	19,31,38,40	0
2	HEM	n	200	43/43	0.99	0.04	10,21,34,37	0
2	HEM	q	200	43/43	0.99	0.04	25,32,42,45	0
2	HEM	v	200	43/43	0.99	0.04	14,24,33,35	0
2	HEM	x	200	43/43	0.99	0.04	10,22,34,38	0
2	HEM	j	200	43/43	1.00	0.03	6,18,36,37	0
2	HEM	k	200	43/43	1.00	0.03	10,21,34,37	0
2	HEM	S	200	43/43	1.00	0.03	8,16,30,33	0
2	HEM	o	200	43/43	1.00	0.04	12,22,37,44	0
2	HEM	L	200	43/43	1.00	0.03	14,21,42,48	0
2	HEM	t	200	43/43	1.00	0.03	10,21,34,37	0
2	HEM	M	200	43/43	1.00	0.03	14,24,43,53	0
2	HEM	g	200	43/43	1.00	0.04	17,29,40,42	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

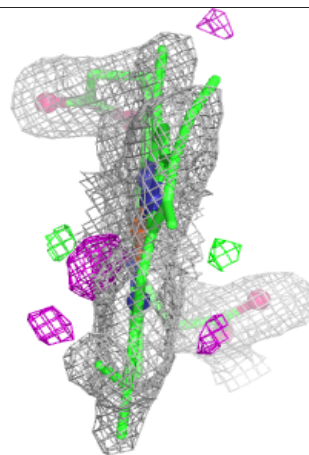
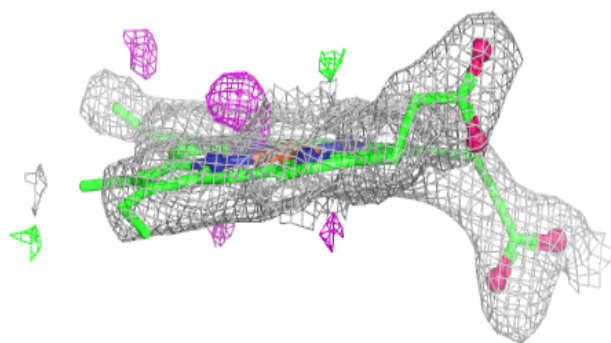
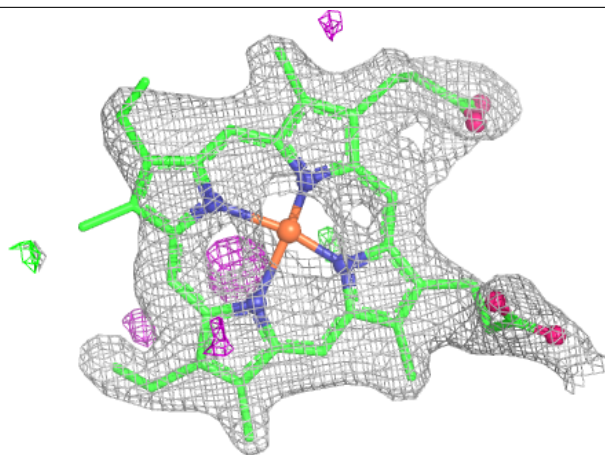
Electron density around HEM B 200:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



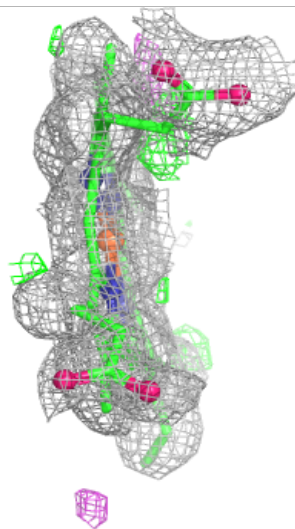
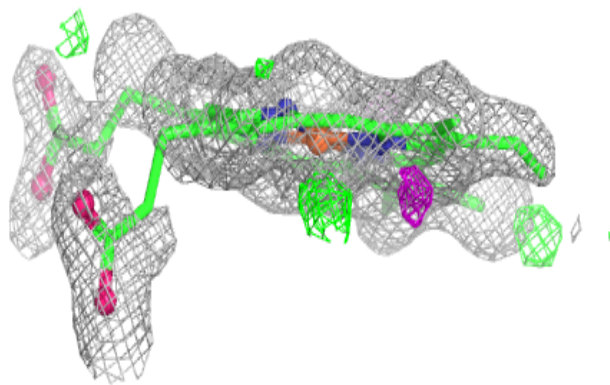
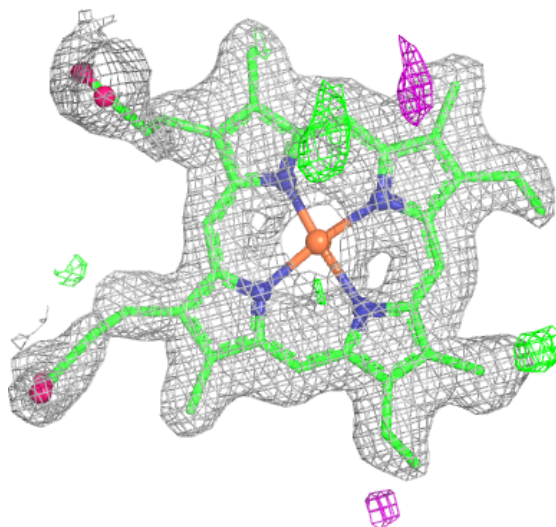
Electron density around HEM C 200:

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and green (positive)



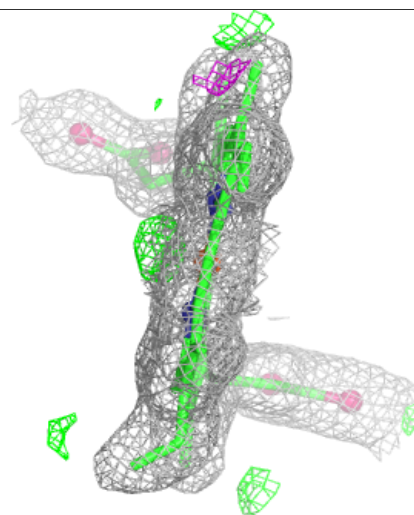
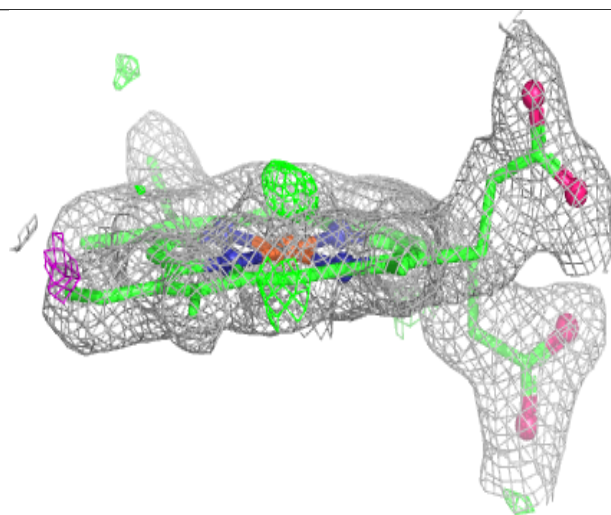
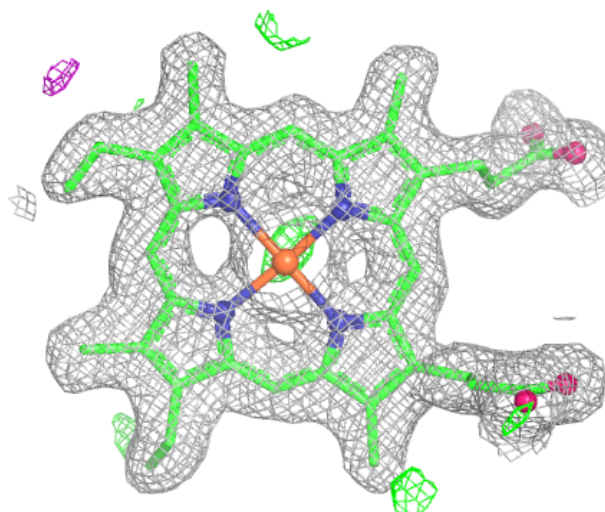
Electron density around HEM F 200:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



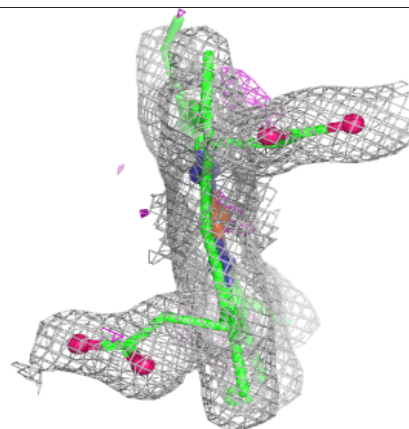
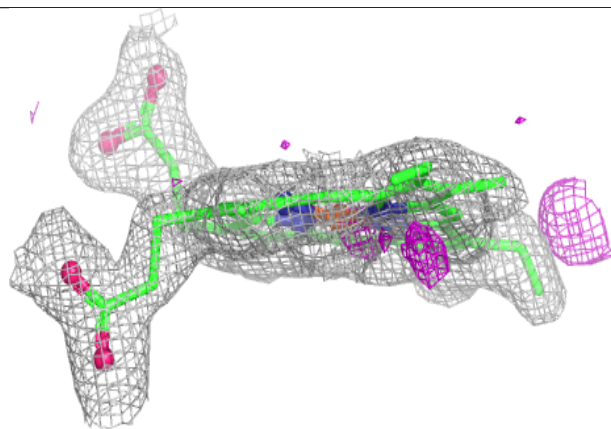
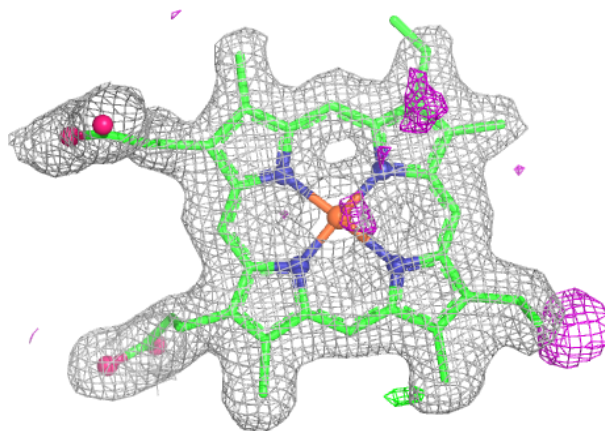
Electron density around HEM H 200:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



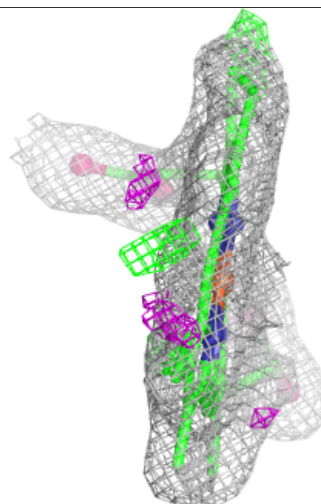
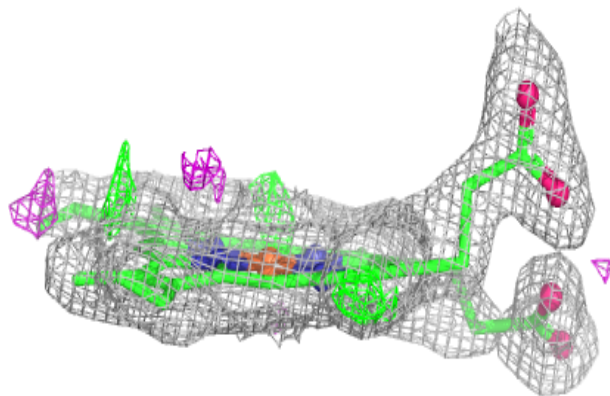
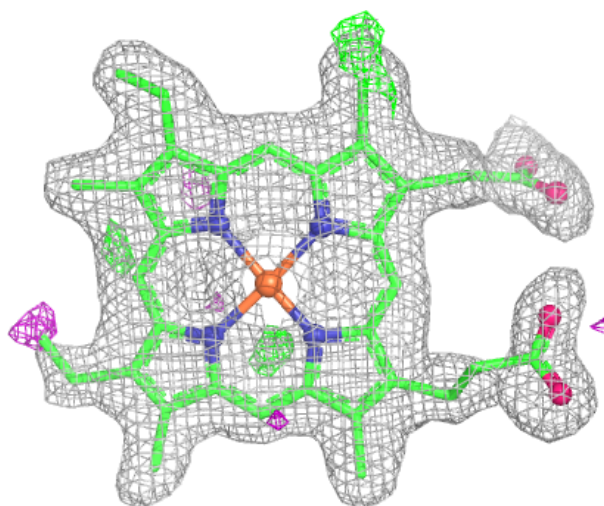
Electron density around HEM I 200:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



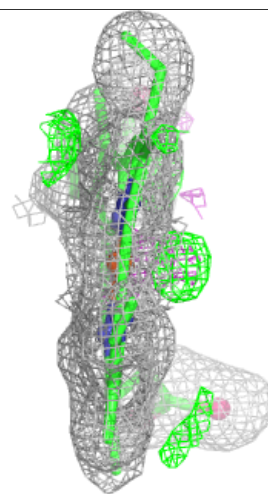
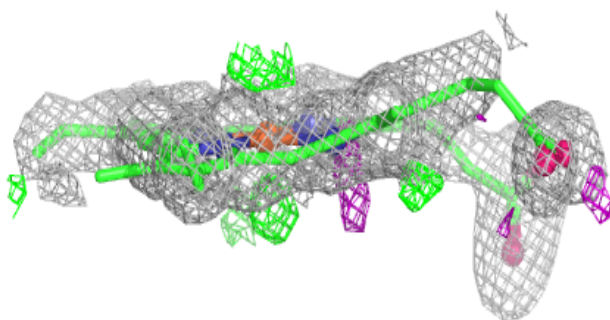
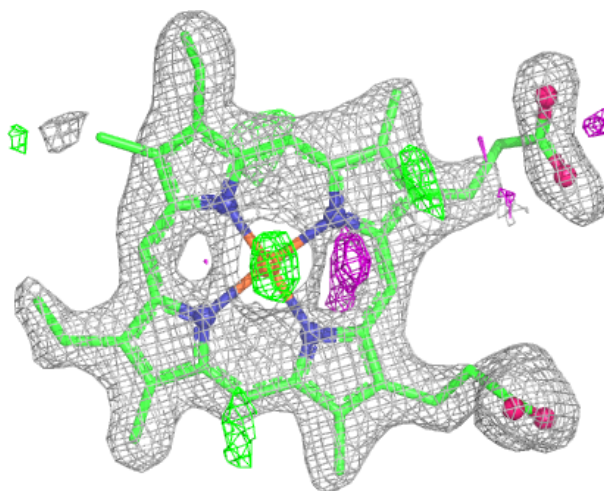
Electron density around HEM P 200:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



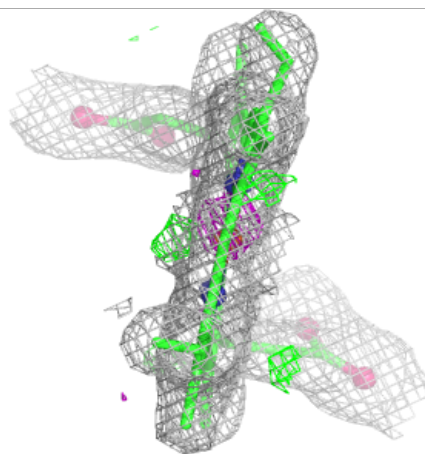
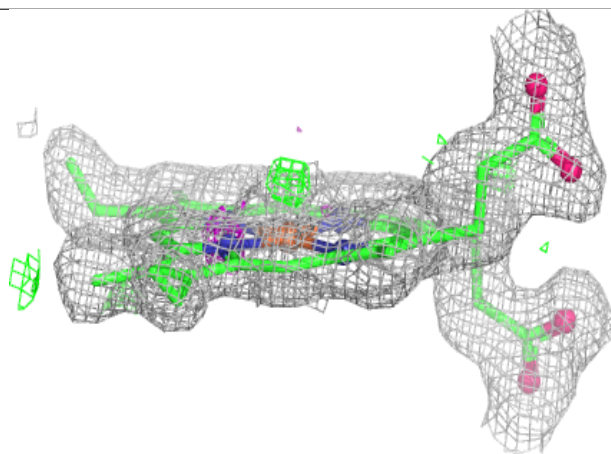
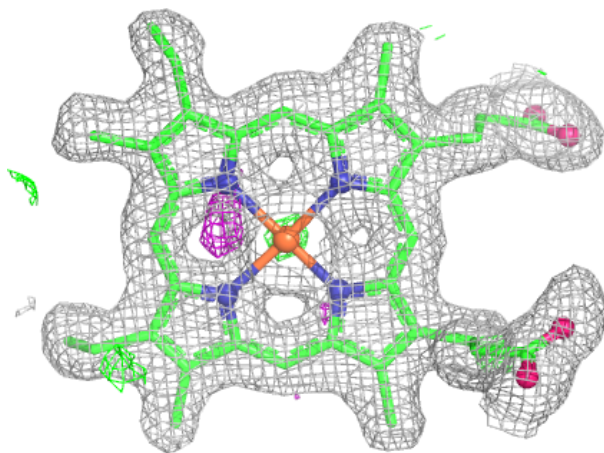
Electron density around HEM R 200:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



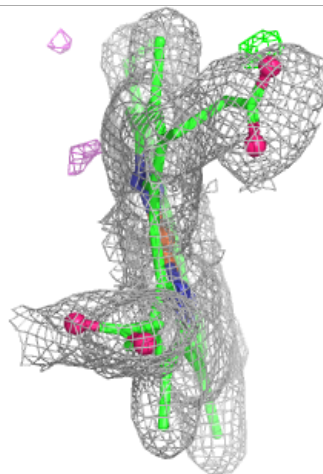
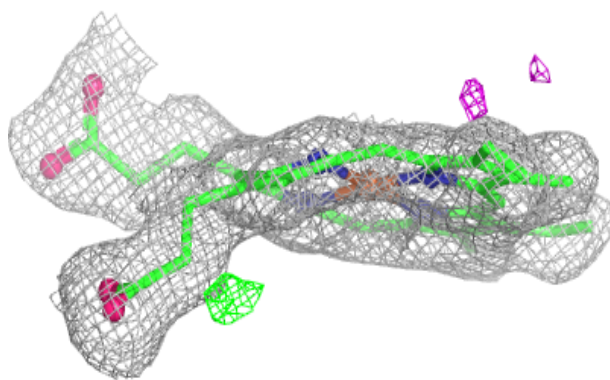
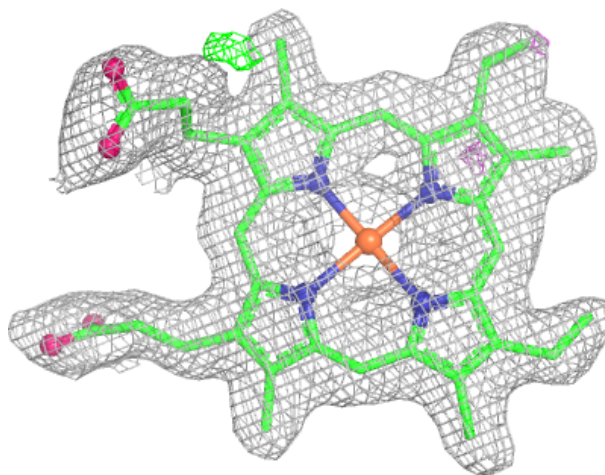
Electron density around HEM U 200:

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and green (positive)



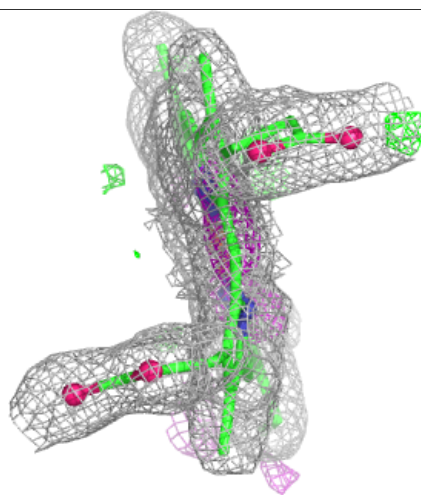
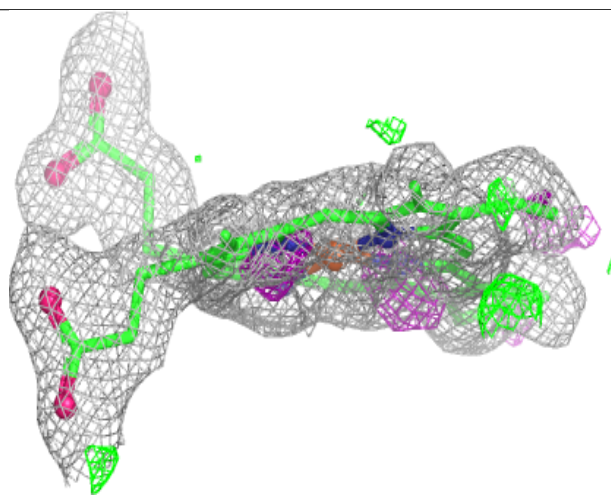
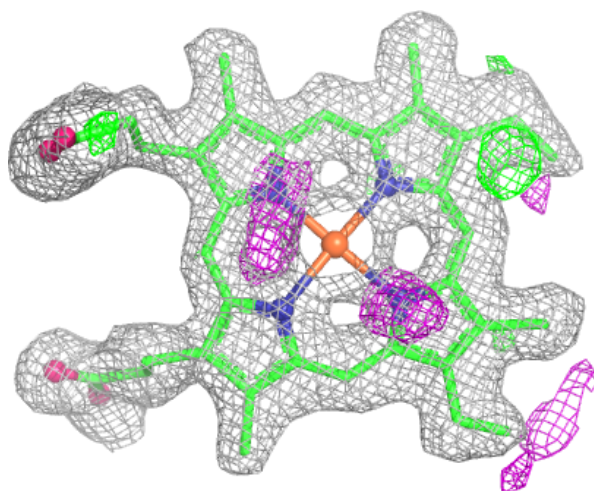
Electron density around HEM X 200:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



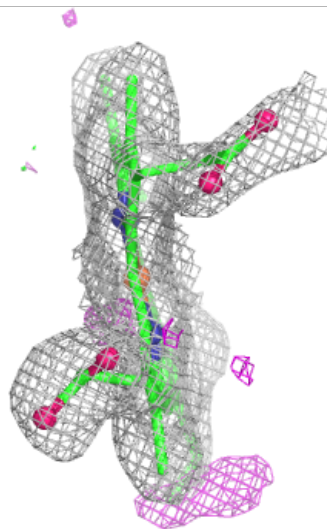
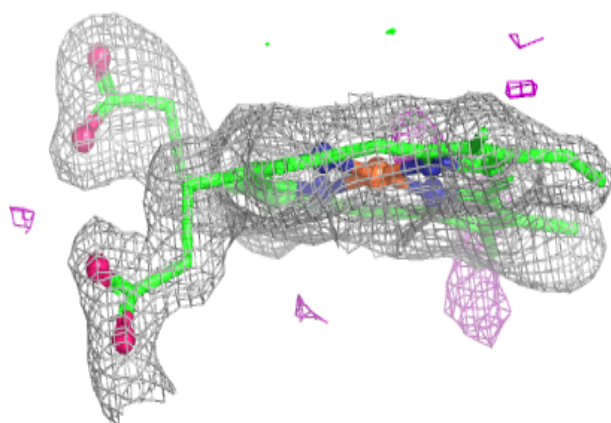
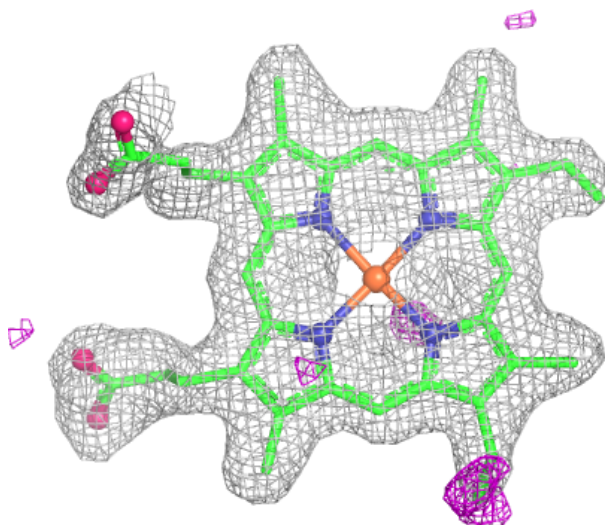
Electron density around HEM a 200:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



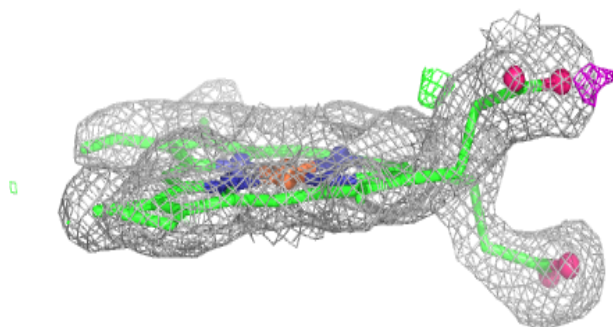
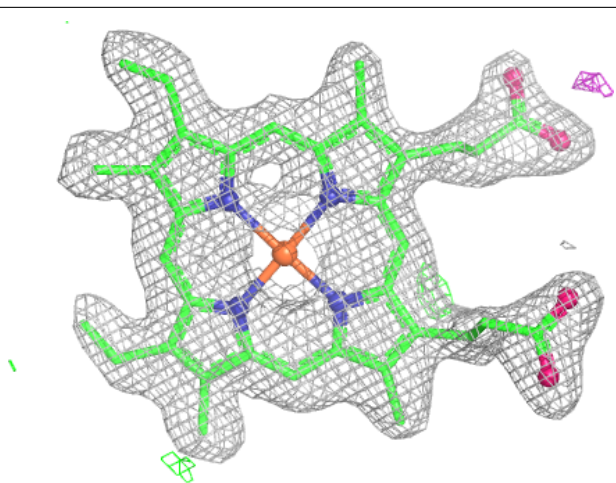
Electron density around HEM c 200:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



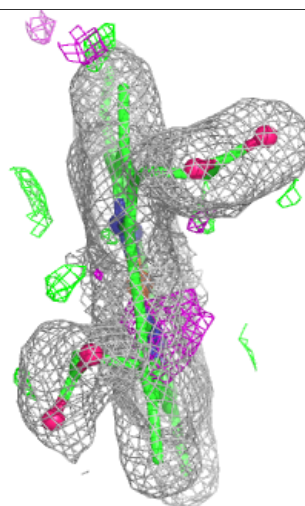
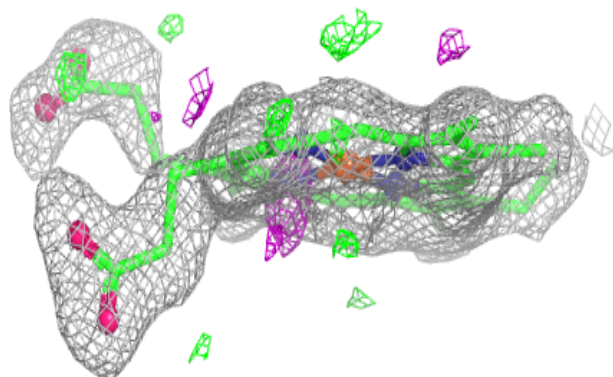
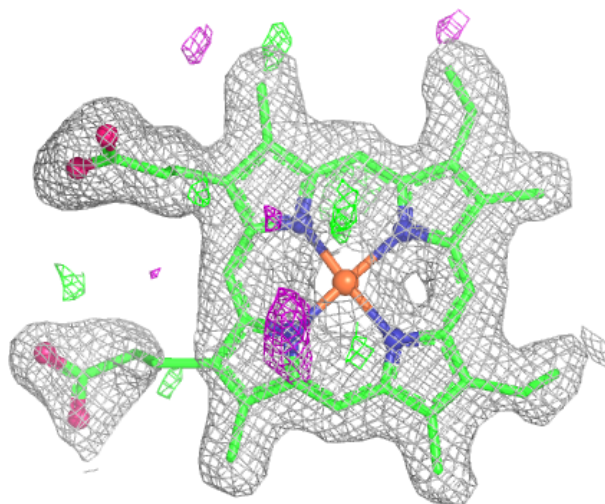
Electron density around HEM e 200:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



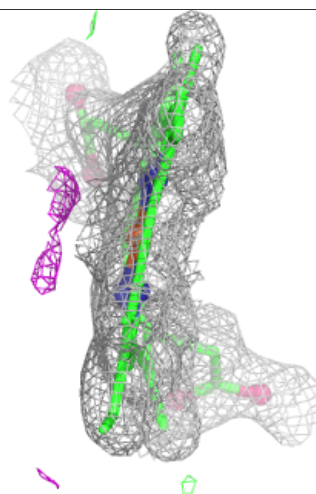
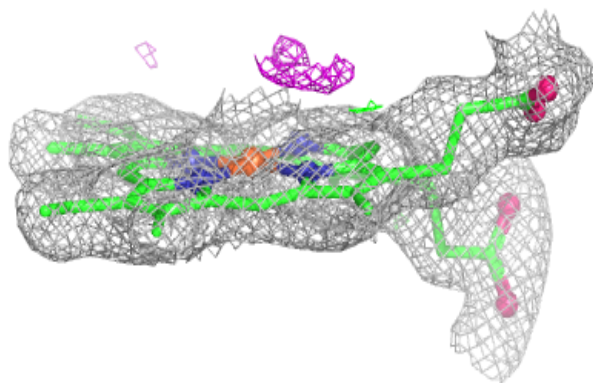
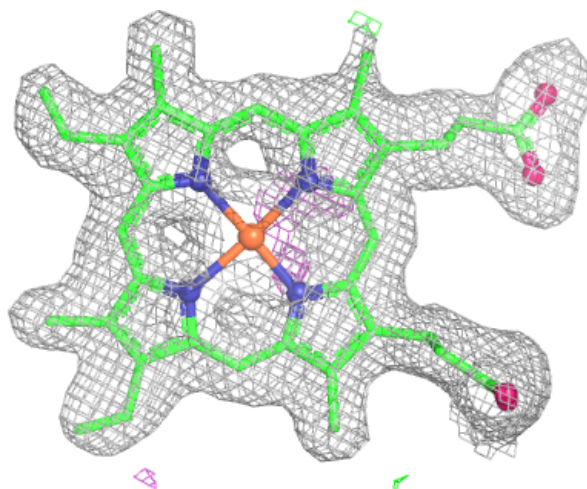
Electron density around HEM n 200:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



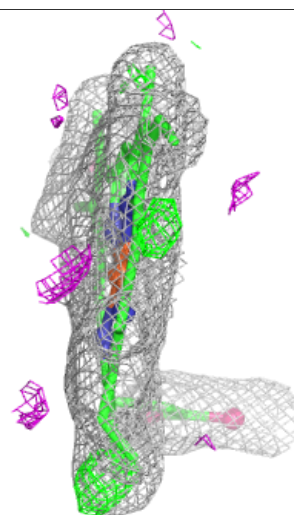
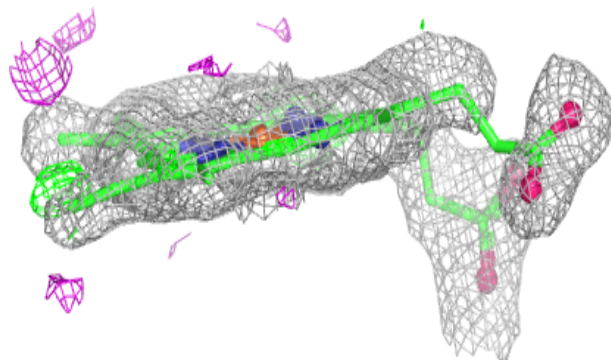
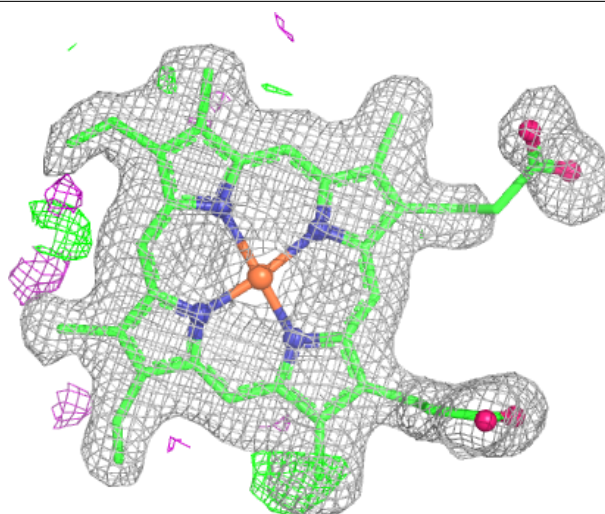
Electron density around HEM q 200:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



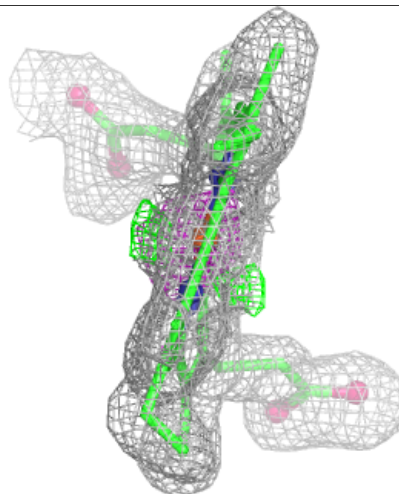
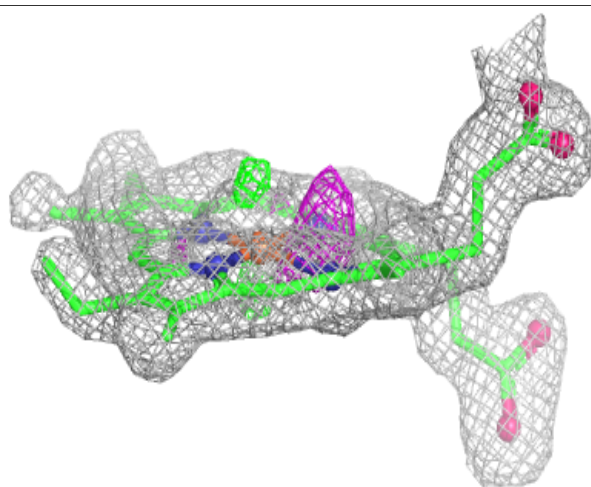
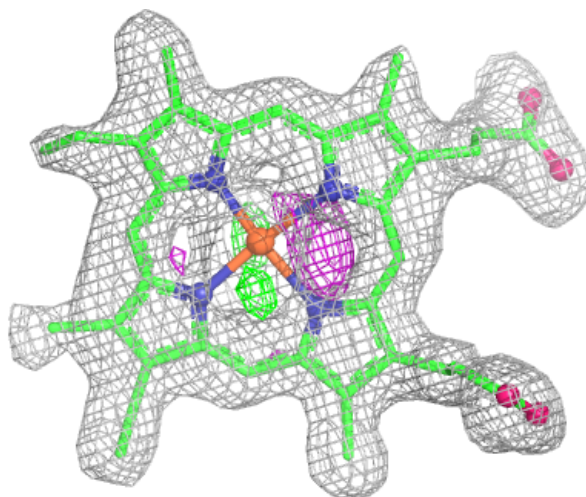
Electron density around HEM v 200:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



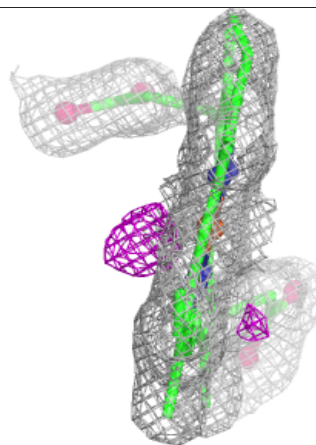
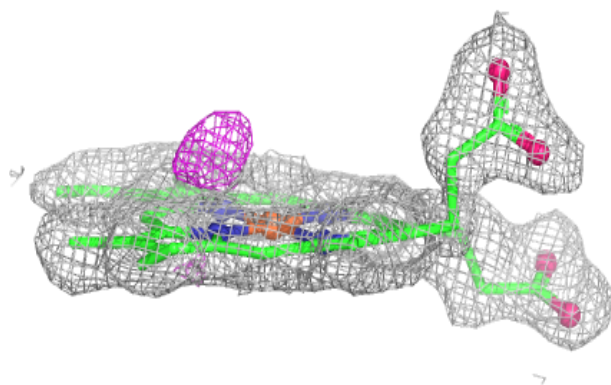
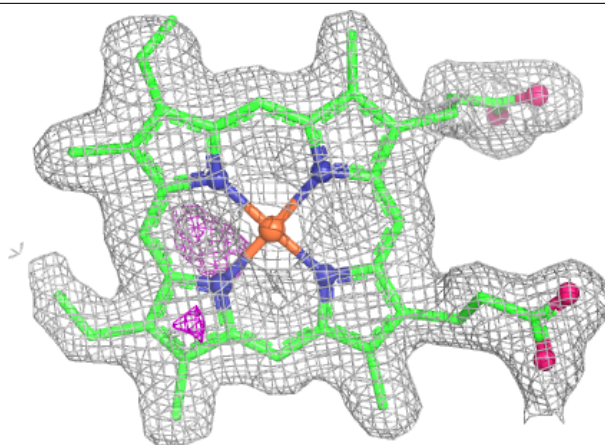
Electron density around HEM x 200:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



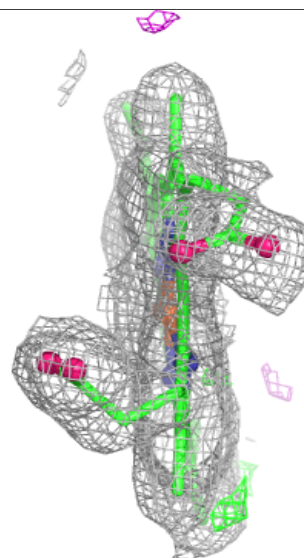
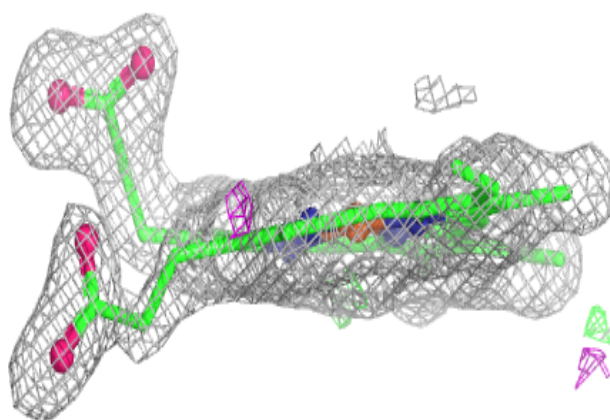
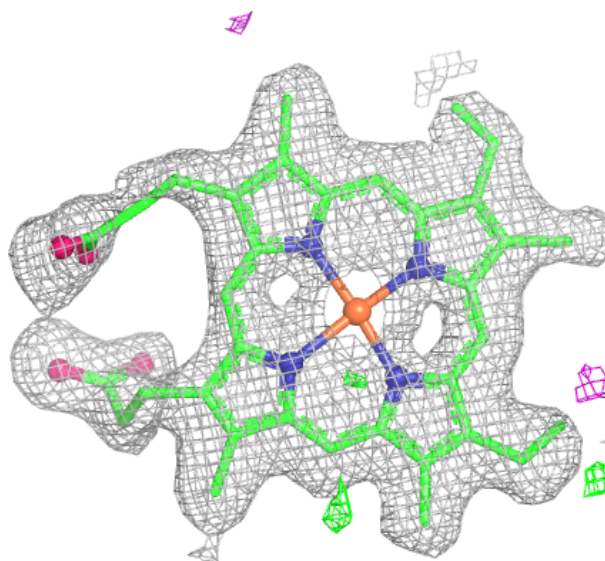
Electron density around HEM j 200:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



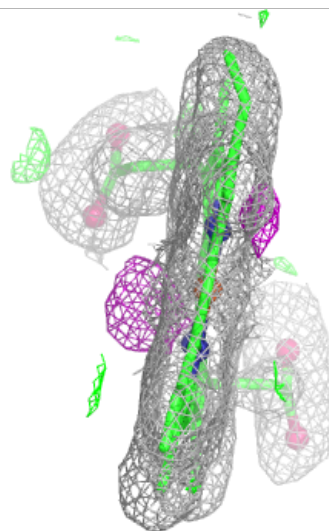
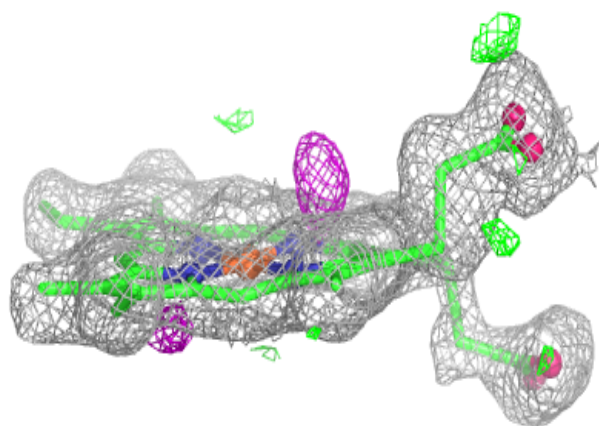
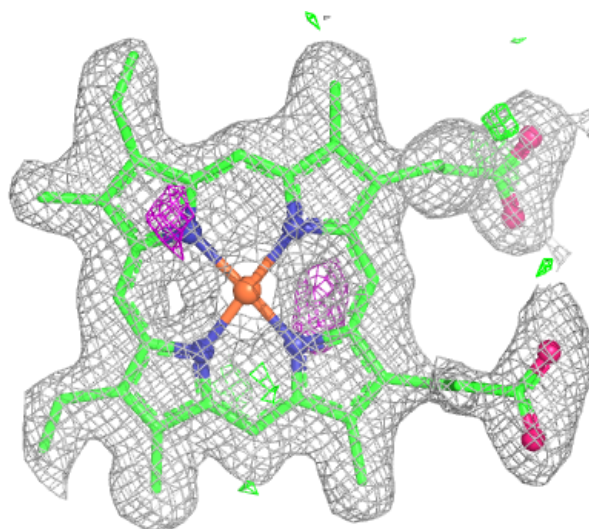
Electron density around HEM k 200:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



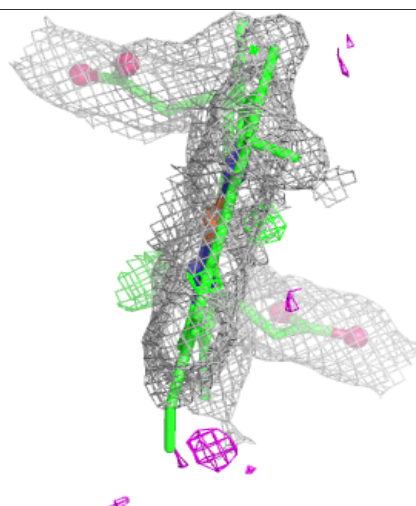
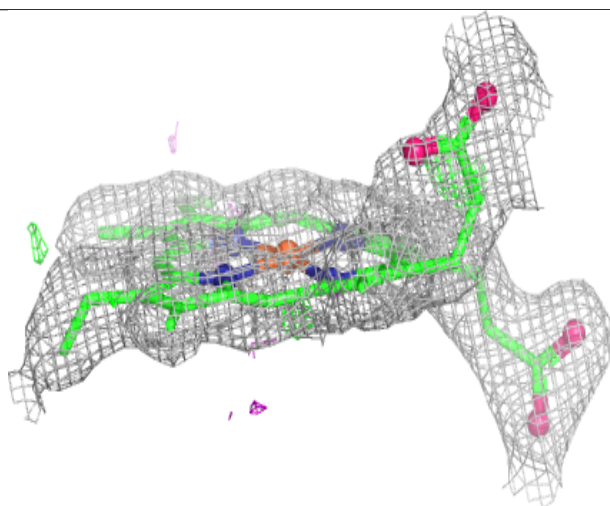
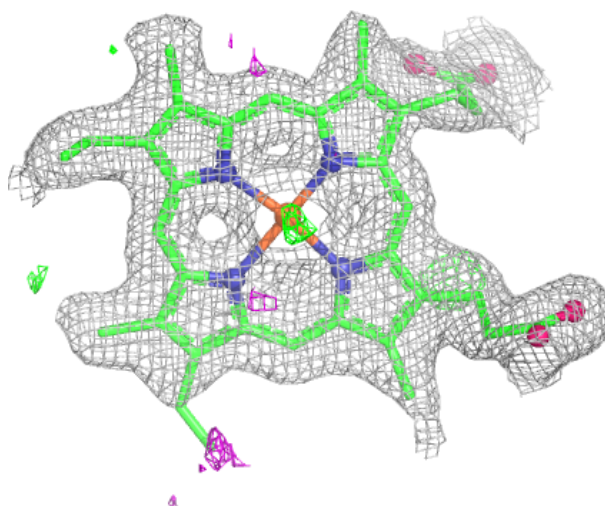
Electron density around HEM S 200:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



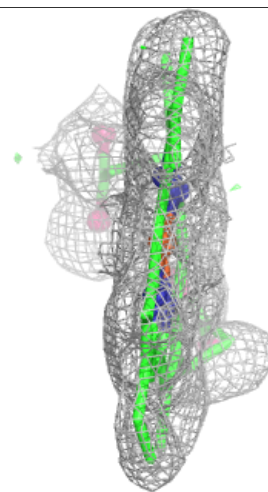
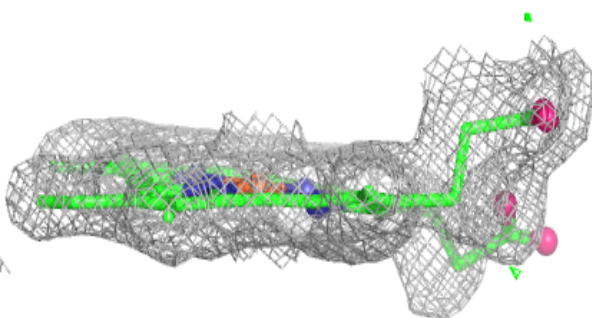
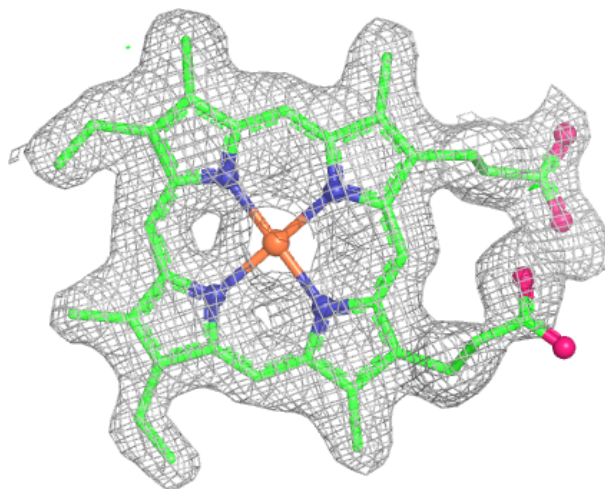
Electron density around HEM o 200:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



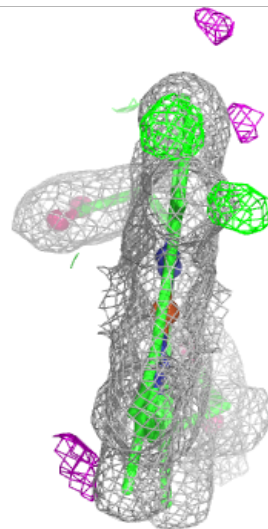
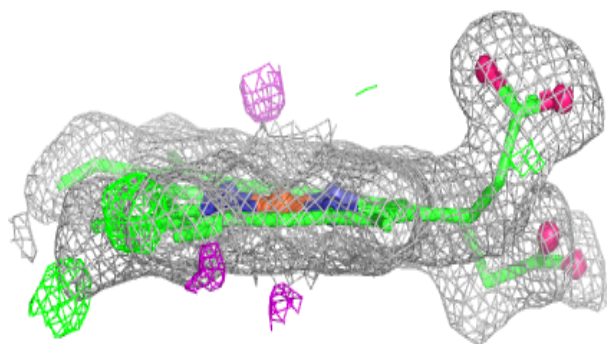
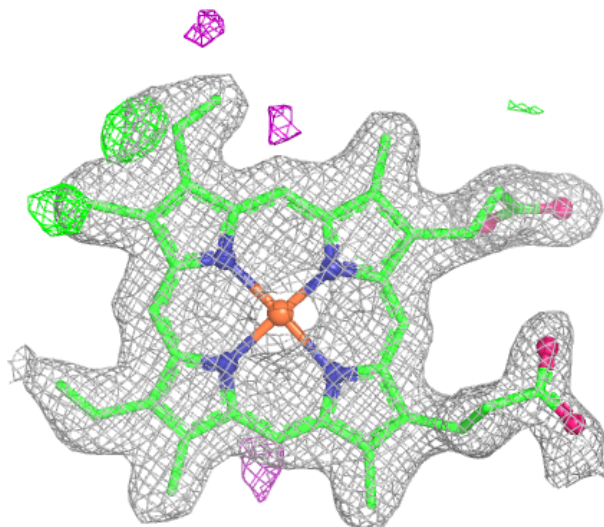
Electron density around HEM L 200:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



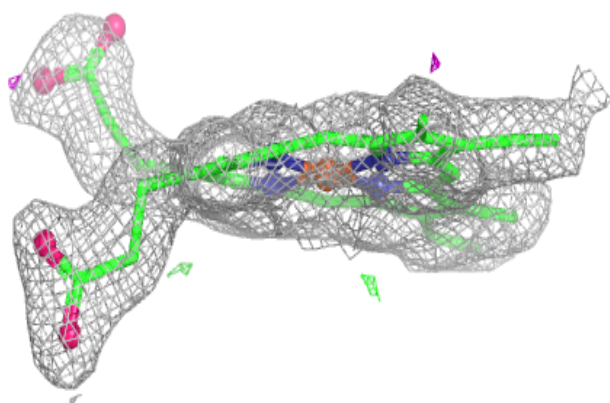
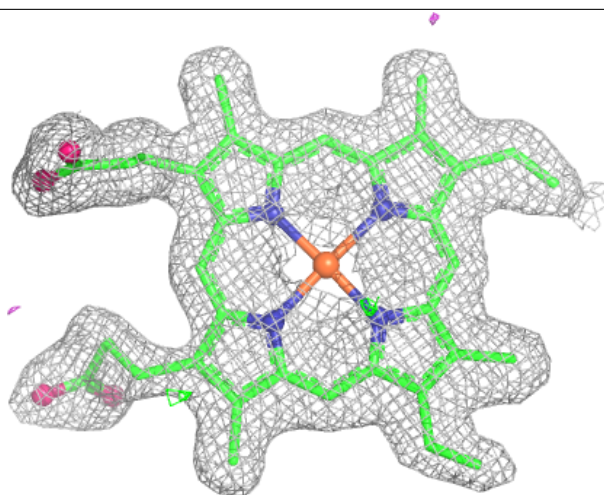
Electron density around HEM t 200:

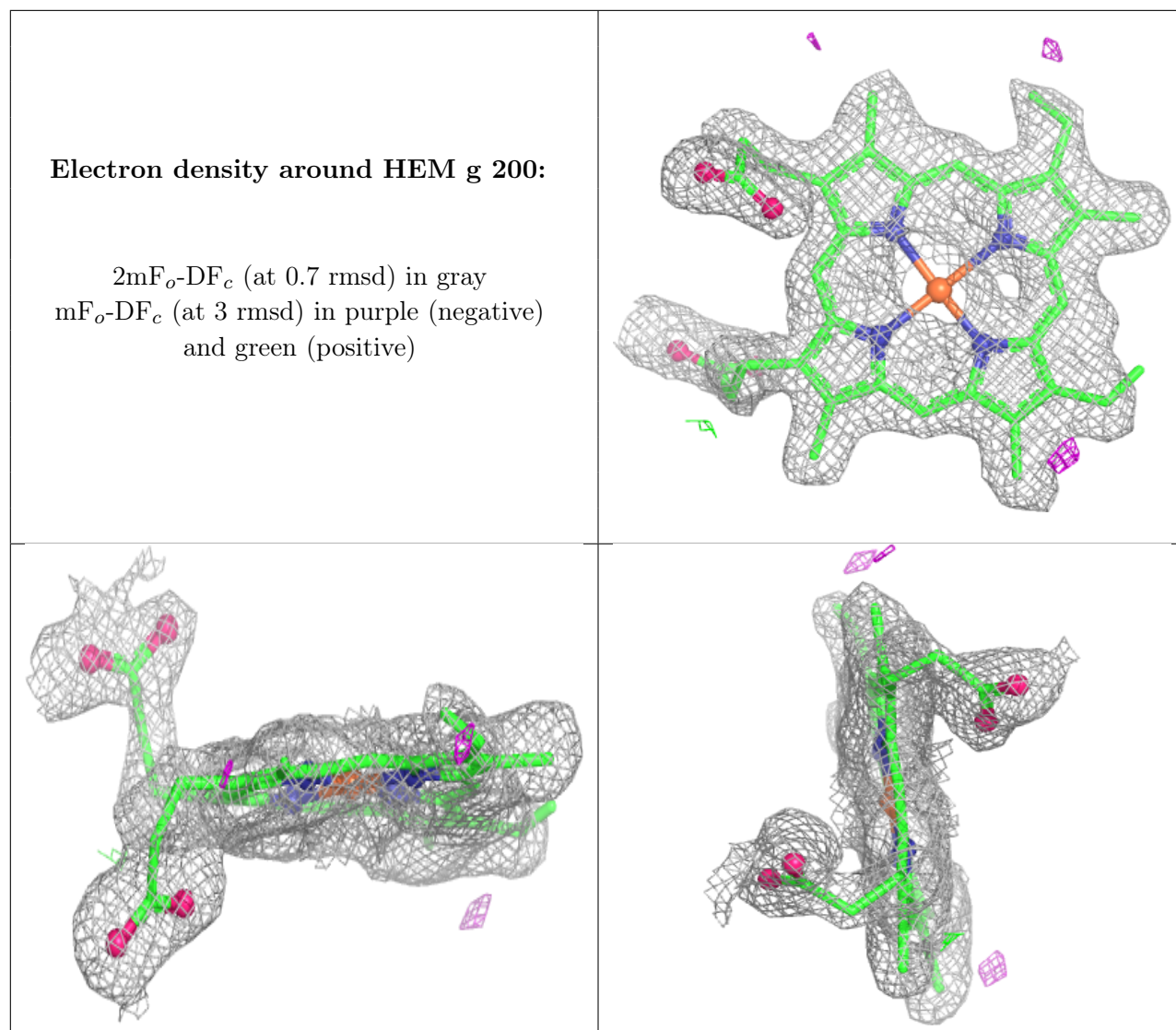
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM M 200:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.